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MEASUREMENTS OF EXHALED BREATH USING A NEW PORTABLE SAMPLING METHOD

by

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ABSTRACT

Breath measurements offer the potential for a direct and noninvasive evaluation of human exposure to volatile organic compounds (VOCs) in the environments in which people live and work. This research study was conducted to further develop the potential of this exposure assessment methodology. A new alveolar breath measurement technique was developed and tested. Air samples were collected in 32 microenvironments and above 6 consumer products to determine a few potential sources of human exposures to selected VOCs. Several people were exposed to the atmosphere in six microenvironments for several hours. Air concentrations of VOCs were measured during these exposures and breath samples were collected and analyzed at multiple time points after the exposure to evaluate elimination kinetics for 21 VOCs. Elimination half-lives were estimated using a mono- and biexponential model. Several other mathematical functions were tested for their ability to accurately describe the breath decay curves for VOCs. The alveolar breath collection and analysis methodology proved to be very useful for collecting many samples in short time intervals and this capability was very important for accurately describing the initial phase of the decay curves. Analysis of microenvironment air samples from homes, businesses, workplaces, vehicles, etc., revealed a wide range of potential sources of human exposures to VOCs at concentrations from 1 to 16,000 $\mu g/m^3$. Breath decay curves were developed over a four hour period after exposure for 21 of 24 target VOCs. A biexponential function provided a better fit for the decay data than did the monoexponential function, suggesting a multi-compartment uptake and elimination model for the human body.

Microg/cu m

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SECTION 1
INTRODUCTION

For nearly a decade, the U.S. EPA has been conducting studies of personal exposure to volatile organic compounds (VOCs) [1-5]. Participants in these studies have also provided breath samples and measured VOC concentrations in breath have demonstrated strong correlations with actual exposure levels. For a few chemicals, e.g. 1,1,1-trichloroethane, trichloroethylene, tetrachloroethylene, *p*-dichlorobenzene, *m*,*p*-xylenes and ethylbenzene, the correlations have been extended further to suggest a link between exposure levels, breath concentrations, and a person's activity or microenvironment [1]. Consequently, two general questions have arisen: (a) what are the common personal activities and microenvironments that may lead to elevated human exposure to VOCs and (b) can breath measurements provide a quantitative measurement of VOC exposure?

The ability to use breath measurements *in lieu* of personal monitoring would circumvent the participant burden experienced with personal monitoring. It would also provide a noninvasive alternative to blood collection and analysis methods for determining body burden. Currently employed models, however, that relate breath to the immediate periods of exposure are imprecise. The VOC residence time in the body is a parameter that is important in perfecting prediction models but is not well described in the literature for nonoccupational situations. Although the breath excretion rates of a few VOCs have been measured in a few subjects [6,7], further information is needed for more compounds, subjects, and exposure levels for the development of accurately predictive models.

A study to further examine the parameters governing breath VOC levels after exposure was sponsored by the U.S. Environmental Protection Agency and is the subject of this report. This research was conducted in three separate phases. First, the feasibility of a device capable of the rapid collection of alveolar breath was studied. The results of these initial investigations are presented in Appendix A. A prototype version of this device was used for breath measurements of individuals exposed to various microenvironments as described in the body of this report. After completion of these microenvironmental exposure studies, the third phase of the research culminated in the design, testing, and construction of a portable alveolar spirometer. This work is described in Appendix B.

The principal objectives of this microenvironmental exposure study were to

a. test the prototype canister based sampling system for measuring VOC concentrations in alveolar breath over short (2 to 5 min) time intervals,

b. examine personal activities and microenvironments commonly encountered by the general population that might lead to elevated VOC exposures,

c. determine the breath VOC concentrations that result from exposure to a variety of different chemicals, and

d. calculate residence times for VOCs in the body, including half-lives and best-fit curve functions, that can be used for developing exposure-prediction models.

In order to achieve these objectives a list of 24 target VOCs was selected covering a wide range of volatilities and chemical functional groups that included halogenated, aliphatic, and aromatic compounds. Approximately 40 microenvironments, consumer products, and human activities were evaluated to determine if they would result in elevated human exposures to the selected VOCs. Specific microenvironments, consumer products, and activities were chosen to represent common sources of exposure in the general population and included stores, businesses, homes, workplaces, swimming pools, automobiles, and solvent containing consumer products. Screening samples were collected and analyzed to determine the identity and levels of the target VOCs associated with these sources.

Based upon the screening analysis results, six microenvironments were chosen for conducting the exposure and breath residence time experiments. The choices were made to include as many target compounds within each microenvironment as possible and to study as many of the 24 target compounds as possible using the six microenvironments. In order to be included in the exposure experiments, the target compound concentrations had to be sufficiently high to provide elevated breath concentrations for decay curve experiments.

Human exposure experiments were conducted in each of the six microenvironments to determine the VOC breath concentration resulting from exposure and subsequent decay in breath levels over a period of several hours. Participants provided a breath sample immediately prior to exposure in the selected microenvironment to determine baseline levels for breath VOCs. They were then exposed to the microenvironment for two to four hours. Eight to eleven breath samples were collected over the four hours after exposure to measure residence times for each elevated compound. Air samples were collected within the subject's microenvironment before, during, and after the exposure to determine intended and unintended exposure concentrations. Experiments within one microenvironment were conducted for four different people to provide some data on the interpersonal variability in breath residence time and decay curve characteristics.

A modified spirometer system capable of collecting alveolar breath canister samples over short time intervals was employed for five of the six microenvironments. This device had been developed and tested during an earlier phase of this research (Appendix A). One advantage of the alveolar spirometer system was the ability to rapidly collect multiple samples after the exposure was completed which allowed for a precise definiton of the early portion of the breath decay curve. Concurrent sample collection using a whole breath spirometer that has been used extensively in previous work [1-8] was conducted during three exposure experiments to allow a side-by-side comparison with the new alveolar system. This whole breath spirometer system was also used for the sixth microenvironment where Tenax cartridges were used to collect those compounds for which canister sample collection and analysis has not been validated.

SECTION 2
CONCLUSIONS

MICROENVIRONMENT AND CONSUMER PRODUCT SCREENING

Air samples were collected in 32 microenvironments and from the headspace above 6 consumer products to identify potential human exposure sources for selected VOCs. Microenvironments were defined as discrete locations where people live, work, or visit with distinct sets of activities or characteristics that affect VOC emissions and airborne concentrations. Examples of the microenvironments sampled in this study included homes, offices, hardware stores, garages, vehicles, and indoor swimming pools. The microenvironmental screening in this research study was directed to find specific target chemicals at sufficiently high concentrations so that human breath concentrations and elimination kinetics after exposure could be examined. The screening also served a broader purpose of increasing our knowledge about VOC pollutant sources and the myriad routes to human exposure.

The concentrations for target VOCs measured in the 32 microenvironments ranged from not detected to 16,000 $\mu g/m^3$. Several locations were found in which several compounds were present at concentrations ranging from 10 to 2000 $\mu g/m^3$. One of the hardware stores was a good example of this type of microenvironment. Other locations had only one or two target compounds present at elevated concentrations. For example, a chloroform level of 600 $\mu g/m^3$ was measured at an indoor swimming pool while the dichloromethane and toluene concentrations at a furniture stripping shop were 5000 and 5700 $\mu g/m^3$ respectively. In some places, for example, a home with moth crystals, p-dichlorobenzene levels remained elevated over long time periods. In other locations, such as in a home garage, short term activities like wood staining and fuel handling increased aliphatic and aromatic hydrocarbon concentrations over a short time period.

Six microenvironments were found that satisfied the exposure study requirement for 21 of the 24 targeted compounds. Microenvironments with sufficiently elevated concentrations of vinyl chloride, carbon tetrachloride, or styrene were not found. Exposure experiments were conducted in a hardware store, furniture stripping shop, indoor swimming facility, wood/metal shop, garage with wood staining and fuel handling, and in a home with moth crystals and wood polish. Each experiment represents a location or activity to which many members of the general population might be exposed. The general results of the screening provide an interesting snapshot of potential VOC exposure possibilities, but one which should not be inferred to all similar microenvironments or activities.

BREATH ANALYSIS AS A MEASURE OF EXPOSURE

The various exposure situations resulted in measureable levels of a wide range of VOCs in the breath. Among the compounds measured in breath were straight-chain aliphatic hydrocarbons, branched-chain aliphatic hydrocarbons, cyclic hydrocarbons, aromatic hydrocarbons, and halogenated hydrocarbons.

The experiments indicated that alveolar breath samples could preserve the time resolution lost in whole breath collection and thus define the very early phases of VOC elimination. Alveolar samples collected with the new device could be obtained within one minute vs. the several minutes required for a whole breath sample using the old spirometer system. This short collection and turn-around time facilitated characterizing the initial portion of elimination decay curves for 18 VOCs in alveolar breath. Analogous data for whole breath provided curves for the same compounds as in alveolar breath with the addition of alpha-pinene, limonene, and p-dichlorobenzene, compounds for which Tenax-based sampling was needed. The alveolar samples often indicated a "second wave" in the decay curves that might be a decay from a second body compartment; such information was not immediately evident from data on whole breath samples. The increased VOC concentrations expected in alveolar samples relative to whole breath samples were not observed. This phenomenon might be related to the slight exertion needed to exhale into a spirometer.

The decay data were mathematically analyzed assuming both a one- and a two-compartment pharmacokinetic model in order to estimate elimination half-lives. In general, the two compartment model provided a better fit to the data as indicated by the F test. One compartment half-lives ranged from 0.08 h for n-nonane to 4.3 h for 1,1,1-tetrachloroethylene. Two compartment half-lives ranged from 0.03 for m,p-xylene to 0.78 h for one dichloromethane measurement for the first half-life and from 0.61 (n-octane) to 11.6 h (vinylidene chloride) for the second half-life. Although the second half-lives were generally less than 8 h, the longest half-life was noted for p-dichlorobenzene, a compound of relatively low volatility known to have a long residence time in the body. The application of generic curve fitting routines to the decay data indicted some promise for modeling the decays for eventual predictive purposes.

The calculated half-lives for a given chemical were examined for trends that might be related to exposure level or study participant. Unfortunately, the data were too limited to make any definitive conclusions to this effect. There appeared to be no dependence of the half-life on exposure level, a conclusion that would make predictive breath studies less complicated in that the exposure level would not need to be considered in the predictive process. The limited data also suggest that the variability of half-life for a particular compound within a single individual is relatively small; the variability among different individuals appeared to be small but more study is needed to verify this conclusion.

QUALITY ASSURANCE

Screening Analysis

No quality control or quality assurance samples were scheduled or collected for this portion of the study. The results were used to select microenvironments for exposure experiments.

Exposure Experiment Samples

Tenax Samples--

The quality control data for analysis of Tenax samples show that the analytical sustem was in control during the entire analysis period. The parameters measured were

daily RRF value for each target analyte,
instrument tune as measured by PFT fragment ions,
system performance characteristics.

The results of the analysis of control samples show consistently high recovery; the data quality objectives were met for all target compounds.

The results of analysis of blanks show that the Tenax used for sampling was uniform and has very low background of target compounds. No spirometer blanks were collected.

The results of the analysis of QA samples was inconclusive. The agreement with the independent laboratory was not good, but the amount of data was very small. Intralaboratory precision, measured as average %RSD between duplicate sample pairs, was very good.

Canister Samples--

The performance of the analytical sustem used to analyze all canister samples was not monitored adequately. Data showing that the system was in control are not available for all analysis days.

Blank and control samples were prepared and anayzed for whole breath and alveolar breath, but not for air samples. No spirometer blanks were collected. For whole breath, recovery was greater than 80% for all compounds except vinyl chloride, n-pentane, 2-methylpentane, n-nonane, and p-xylene. For alveolar breath, recovery was greater than 80% for all compounds except 2-methylpentane and benzene. The results of analysis of blanks show low background of all target compounds, except for the alveolar breath blank, experiment FS1.

No duplicate samples were analyzed by an independent laboratory. Intralaboratory precision was very good for most analytes. The results of the analysis of performance evaluation samples (2 canisters) show a high negative bias.

SECTION 3
RECOMMENDATIONS

SAMPLE COLLECTION AND ANALYSIS

During this research study, further experience was gained in using canisters for collection and direct GC/MS analysis for exhaled human breath. A modified spirometer designed for sampling alveolar breath was used for the first time. The following recommendations are suggested to further improve this methodology:

1. Miniaturize the alveolar spirometer system so that it can be carried by hand and simplify the design so that it can be widely employed for environmental and industrial hygiene exposure measurements.
2. Field test a miniaturized version of the alveolar spirometer and correct any problems before its use in larger studies.
3. Prepare all breath calibration and control standards with humidity and carbon dioxide levels that are comparable to those in human breath. Instrumental responses may be significantly affected by the presence of these breath constituents.
4. Examine the feasibility of expanding the analyte list for very volatile compounds such as ethane and acetylene that may be found in breath. The chromatographic separation and mass spectral analysis methodology may need modification for these compounds.
5. Examine the feasibility of expanding the analyte list for polar organic compounds in breath. The method of sample drying and introduction will need modification for effective analysis of polar analytes.

MICROENVIRONMENT SCREENING

We recommend that screening of the wide variety of microenvironments and consumer product emissions for VOCs be continued in future studies. Further examination of the microenvironments in which people spend much of their time can fill in gaps in our knowledge about the magnitude and sources of human exposure to VOCs.

FURTHER DATA ANALYSIS

Data collected during this study should be analyzed further to maximize the information gained from this work. Recommendations are listed below.

1. Additional mathematical modeling should be performed. The use of a three compartment pharmacokinetic model could be applied to see if there is practical importance for these volatile compounds. Additional information might be obtained from this sort of analysis for the less volatile p-dichlorobenzene and limonene. More complex functions, such as polynomials and other equations of higher order should be applied to the data to further define the shape of the curve. Careful attention should be paid to trends among compound class.
2. The half-lives calculated in this project should be compared to those available from previous work. The method by which breath was collected should be an important consideration in making comparisons.

FUTURE EXPERIMENTS

Several experiments can be envisioned that would advance the predictive ability of breath measurements. Such work should include:

1. Decay curves and half-lives should be measured using multiple exposures to a variety of exposure concentrations. The experiments should help define intraindividual variability and any dependence of the half-life on the exposure level. Experiments should be performed on individuals chosen to reflect different, types of people e.g., body builds, weight, etc. in the general population. Such a study would also define interindividual variability. The number of compounds targeted should be increased so that additional decay information is obtained.
2. The importance of various physiological parameters on the measured decays and half-lives should be determined. Such factors include body build, physical activity during exposure, and the effect of breathing technique during sample collection. The effect of such parameters on the measured half-life and blood:breath partition ratio will have profound effects on the utility of breath measurements as predictors of exposure. The effect of the time at which

the breath is sampled after the end of the exposure should be studied because the apparent blood/breath ratio might be expected to change as different body compartments clear. Again, this is extremely important for predicting exposure based on breath measurements.

3. The effect of the exposure time on the half-life and partition ratio should be determined under constant exposure levels. Changes in the values as the exposure time changes will reflect the equilibration of different body compartments to differing extents. These experiments will help define the optimal time after the exposure to make the breath measurement. That is, the post exposure sampling time will define which compartment decay is being measured.
4. Studies testing the predictive abilities of the developed models should be performed using participants not involved in the above experiments. Based on breath measurements for a range of compounds, the exposure level should be predicted and compared to the measured air level.

QUALITY ASSURANCE

1. The canister loading/instrument calibration procedures need to be reviewed and revised.
2. The usefulness of QC checks for the canister analytical system should be reviewed. Priority should be given to development of QC checks and control limits.
3. Insufficient quality control and quality assurance samples were scheduled for the exposure study (canisters). Blanks and controls should be scheduled for each matrix/sampling devise combination. Results of analysis of duplicate samples by an independent laboratory provides important precision estimates than cannot be obtained by intralaboratory analysis of duplicates. Analysis of canister samples should be included in the interlaboratory program.
4. Two ions, at least, should be utilized for the identification of target analytes by GC/MS. This is an essential QC check for all Tenax data, and similar procedures should be developed for analysis of canister samples.

SECTION 4
SAMPLE COLLECTION AND ANALYSIS

INTRODUCTION

Sample collection activities were divided into two phases during this research project. First, screening samples were collected to evaluate VOC concentrations and emissions from a large number of microenvironments and consumer products. Results of the screening sample analyses were used to select exposure environments for the breath decay experiments. Screening samples were collected with both canisters and Tenax cartridges, followed by GC/MS analysis. In the second phase, exposure experiments were conducted in which both breath and air samples were collected to determine the exposure level, the breath concentration after exposure, and the decay in breath concentration over time. Alveolar canister breath samples were collected in nine of the ten exposure experiments while whole breath canister samples were collected concurrently in three of those experiments. Canister air samples were collected before, during, and after participant exposure in each experiment to determine the exposure concentration and any possible confounding exposure to the selected compounds outside of the chosen microenvironment. Tenax cartridges were used to collect whole breath and air samples during the tenth exposure experiment in which the target compounds had low volatility or had not been previously validated for canister collection and analysis. All exposure experiment samples were analyzed by GC/MS.

COLLECTION OF SCREENING SAMPLES

Screening Sample Collection Procedures

Both canisters and Tenax cartridges were used to monitor target VOC concentrations (Table 4-1) in numerous microenvironments. These microenvironments were selected as areas or activities that might provide VOC exposures to portions of the general population. They included homes, offices, vehicles, light industry, and commercial establishments. Several microenvironments were located on the RTI campus or at the homes, vehicles, and garages to which RTI employees had access. Many other

TABLE 4-1. TARGET CHEMICALS FOR SCREENING AND BREATH EXPOSURE STUDY SAMPLES

Compound	Canister	Tenax
Vinyl chloride	✓	
Isopentane	✓	
Vinylidene chloride	✓	
n-Pentane	✓	
Dichloromethane	✓	
2-Methylpentane	✓	
Chloroform	✓	
1,1,1-Trichloroethane	✓	
Carbon tetrachloride	✓	
Benzene	✓	
Trichloroethylene	✓	
n-Octane	✓	✓
Toluene	✓	
n-Nonane	✓	
Tetrachloroethylene	✓	
Ethylbenzene	✓	
p-Xylene (or *m*-)	✓	✓
Styrene	✓	
o-Xylene	✓	✓
α-Pinene		✓
n-Decane	✓	✓
Limonene		✓
p-Dichlorobenzene		✓
n-Dodecane		✓

microenvironments were commercial or municipal establishments, and special permission was secured for collecting screening samples in these areas. A copy of the consent form used to gain entry to these establishments is presented in Appendix C. Establishment confidentiality was assured in all cases.

In most microenvironments, an evacuated canister was simply opened and allowed to fill to ambient pressure in under one minute. A data sheet was used to record activities, apparent ventilation, establishment volume, characteristics, and other information that might be useful for evaluating analytical results. Some activities required sample collection over time intervals ranging from several minutes to several hours. For long exposure times, a fixed needle orifice of a selected diameter was attached to the canister inlet to regulate the flow rate. These samples were slightly time-weighted since the sampling flow rate decreased after the canister reached 50% of ambient pressure. All canister samples were stored sealed at room temperature until analysis.

Fixed-site air samples were also collected at three locations by pulling air through a 6.0 x 1.4 cm i.d. bed of Tenax GC contained in a glass tube using a constant flow pump (DuPont Model P125A). Preparation of these cartridges followed an extremely rigorous procedure, described in detail in a standard operating procedure [8] to ensure minimal organic contamination of the sorbent cartridge. Glass fiber filters (Gelman, 25 mm) were attached to the inlet end of the Tenax cartridge to remove particulates from the sampled air. For fixed-site air sampling, the pump and cartridge were placed inside a metal box for protection, with only the inlet end of the sample cartridge protruding. Tenax cartridges were stored in sealed cans in a solvent-free environment at all times, except during actual sample collection. Tenax cartridges were used to collect less volatile compounds such as p-dichlorobenzene and n-dodecane and compounds that have not been previously validated for canister collection and analysis, including α-pinene and limonene.

Two target compounds, limonene and α-pinene, were not found in any microenvironment at concentrations sufficiently elevated for conducting exposure experiments. These compounds were believed to be common ingredients of a number of deoderizers and home cleaning products. Several such products were selected based on their listed ingredients or claims of pine or lemon scent. They were tested for emissions of both α-pinene and limonene. Emission samples were collected using a dynamic headspace purge apparatus described in Figure 4-1. The headspace samples were collected for qualitative analysis only. Sample collection conditions were not tightly controlled but in general the product temperature ranged from 30° to 40°C and headspace was purged with helium at a flow rate ranging from 20 to 50 mL/min for 10 to 15 minutes. The headspace was swept through a Tenax cartridge which was analyzed by GC/MS to determine the approximate amount of α-pinene and limonene.

Screening Sample Collection

Canister screening samples were collected in the 32 different microenvironmental locations listed in Table 4-2. The microenvironments included homes, businesses, garages, repair shops, vehicles, etc. These particular microenvironments were chosen for two reasons. First, most locations were chosen because it was hypothesized that a particular compound or group of compounds might be present. For example, chloroform should be present at high concentrations at the swimming pool while the refueling experiment was chosen for the aliphatic and aromatic compounds that should be present in gasoline. Each microenvironment and the rationale for its inclusion will be described in Section 6 of this report along with a discussion of the screening results. Second, a large part of the general population has potential exposure to these or similar microenvironments. A few were opportunistic sample collections, for example a laboratory that had recently been re-roofed in which a strong asphalt odor was noticed.

Three of the microenvironments sampled using canisters were also sampled using Tenax cartridges. Tenax was used to collect samples in the furniture stripping shop, a hardware store, and in a woodworking shop (Table 4-3) to determine if elevated levels of α-pinene and/or limonene were present. These three areas were thought to be excellent candidates for emissions of these compounds since all three dealt in wood products and wood finishes. Samples of air at these three locations were collected over a four hour period and analyzed to determine the approximate concentrations of Tenax target compounds. Six consumer products (Table 4-4) were obtained at a local grocery store and tested for emissions of α-pinene and limonene

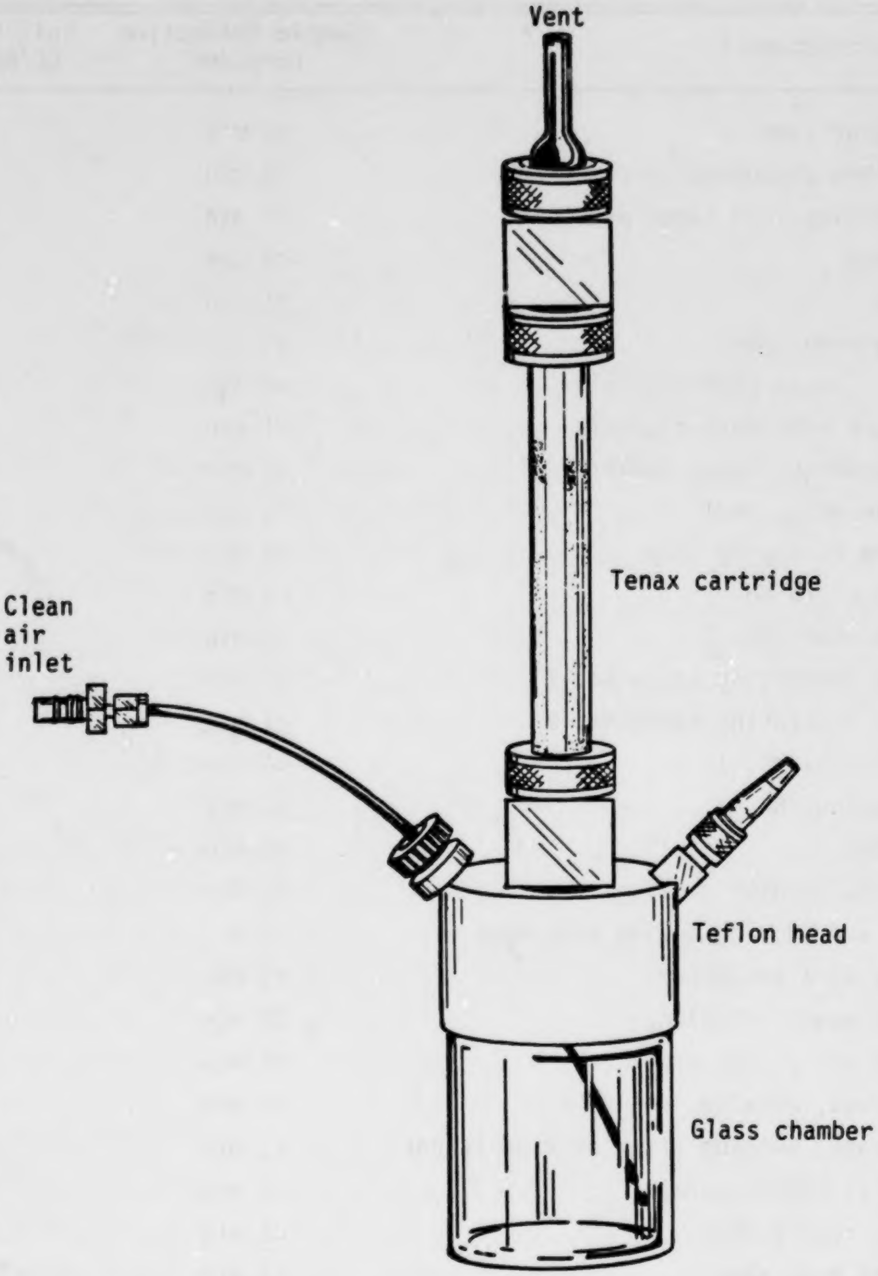
Vent
Tenax cartridge
Clean
air
inlet
Teflon head
Glass chamber

Figure 4-1. Dynamic headspace purge apparatus for measuring consumer product emissions.

TABLE 4-2. MICROENVIRONMENT SCREENING SAMPLE LOCATIONS FOR CANISTER AIR SAMPLING

Microenvironment	Sample Collection Duration	Full Scan or MID[a] GC/MS Analysis
Photocopier room	<1 min	FS
High volume photocopy/print center	<1 min	FS
Room painting (oil based paints)	<1 min	FS
Metal shop	<1 min	FS
Woodshop	<1 min	FS
Wood staining area	<1 min	FS
Home No. 1 with moth crystals	<1 min	FS
Home No. 2 with moth crystals	<1 min	FS
Office with one heavy smoker	<1 min	FS
Indoor swimming pool	<1 min	FS
Furniture stripping shop	<1 min	FS
Hardware store No. 1	<1 min	FS
Hardware store No. 2	<1 min	FS
Interior decorating store No. 1	<1 min	FS
Interior decorating store No. 2	<1 min	FS
Beauty school No. 1	<1 min	FS
Beauty school No. 2	<1 min	FS
Laundromat	<1 min	FS
Bar/nightclub with smoking	<1 min	MID
Driving and smoking during rush hour	1 h	MID
Outdoors at a truckstop	<1 min	MID
Auto and mower refueling	20 min	MID
Inside a new pickup truck cab	<1 min	MID
Home garage, morning	<1 min	MID
Home garage, evening after driving in car	<1 min	MID
Commercial repair garage	<1 min	MID
Body and repair shop	<1 min	MID
Paint and body shop	<1 min	MID
Home with diapers soaking in bleach	12 h	MID

(continued)

TABLE 4-2 (cont'd.)

Microenvironment	Sample Collection Duration	Full Scan or MID[a] GC/MS Analysis
Mass spectrometer laboratory facility	<1 min	MID
Laboratory recently re-roofed	<1 min	MID
Packaging facility with much styrofoam	<1 min	MID

[a] FS = full scan, MID = multiple ion detection.

TABLE 4-3. MICROENVIRONMENT SCREENING SAMPLE LOCATIONS FOR TENAX AIR SAMPLING

Microenvironment	Sample Collection Duration
Furniture stripping shop	4 h
Hardware store No. 1	4 h
Wood shop	4 h

TABLE 4-4. CONSUMER PRODUCT EMISSION SAMPLES COLLECTED ON TENAX USING A DYNAMIC HEADSPACE PURGE

Product Name	Test Temperature	Headspace Volume Analyzed
Pine-Sol® (19% pine oil)	40°C	0.23 L
Airwick® Solid Room Deoderizer (lemon scent)	30°C	0.45 L
Wood Plus® Polish (lemon scent)	30°C	0.48 L
Johnny Fresh® Bathroom Bowl Cleaner (pine scent)	26°C	0.30 L
Old English® Furniture Polish	26°C	0.23 L
Renuzit Roomate® Liquid Air Freshner	26°C	0.22 L

after elevated concentrations of these two compounds were not found in any microenvironment. Headspace samples collected on Tenax were analyzed to determine if the compounds were present and, if so, the amount relative to the other products. Potential interfering compounds were also examined in the headspace samples.

Quality control samples, including blanks, controls, and duplicate samples were not employed during screening sample collection and analysis activities. Analytical instruments were calibrated using single concentration calibrations for both canister and Tenax screening analyses. The sample concentrations reported in Section 6 for screening samples should be used as close approximations. The screening sample data were used only to select microenvironments and were not used to evaluate actual exposure concentrations.

COLLECTION OF EXPOSURE EXPERIMENT SAMPLES

Selection of Exposure Microenvironments

Exposure experiments were conducted to measure participant breath levels of VOCs after spending time in selected microenvironments. A second goal was the measurement of breath clearance rates of different VOCs from the body after the participant left the exposure microenvironment. Several microenvironments were chosen for conducting the exposure experiments based on the identities, number, and concentrations of target VOCs detected during screening experiments. Each chemical had to have sufficiently high exposure levels so that the participant's breath concentration was still measureable several hours after leaving the exposure site.

Six microenvironments were selected as sites for exposure experiments to measure breath concentrations and clearance rates. These sites were the furniture stripping shop, hardware store no. 1, wood and metal shop, swimming pool, garage with fuel handling and wood staining, and a home with moth crystals and furniture polish. The chemicals targeted for each microenvironment are listed in Table 4-5. The targeted chemicals were found at each microenvironment, except for the less volatile aliphatic hydrocarbons in the wood and metal shop. An absence of freshly stained wood was the most likely reason the concentrations of aliphatic compounds in the wood and metal shop air were lower than those measured during screening. All of the microenvironments except the swimming pool had

TABLE 4-5. MICROENVIRONMENTS AND CHEMICALS SELECTED FOR BREATH EXPOSURE EXPERIMENTS

Microenvironment	Intended Target Chemicals
Furniture stripping shop	Dichloromethane, toluene, 1,1,1-trichloroethane, other aromatic and aliphatic hydrocarbons
Hardware store no. 1	Dichloromethane, 1,1,1-trichloroethane, tetrachloroethylene, aliphatic and aromatic hydrocarbons
Indoor swimming pool	Chloroform
Wood and metal shop	Less volatile aliphatic hydrocarbons, 1,1,1-trichloroethane, vinylidene chloride
Home garage with fuel handling and wood staining	Very volatile and less volatile aliphatic hydrocarbons, aromatic hydrocarbons including benzene
Home with consumer products (moth crystals and wood polish)	Limonene, α-pinene, p-dichlorobenzene

multiple target compounds at elevated concentrations. Decay curves were obtained for all target compounds except vinyl chloride, carbon tetrachloride, and styrene. Sufficient resources remained after the first six microenvironment experiments to perform repeat experiments at one location. The hardware store was chosen as the location for repeat experiments. A total of four different participants were exposed in the hardware store at three different times. On two of those occasions, two participants were exposed at the same time and breath samples were collected simultaneously. These repeat experiments were conducted to examine interpersonal variations in breath decay curves. Examination of intrapersonal variability was made possible because a participant may have been exposed to the same chemical in more than one exposure experiment.

Description of Exposure Experiments

Each breath exposure experiment was conducted to determine a participant's breath concentration of one or more target chemicals after spending time in an area with a measured air concentration of the same chemical(s). An air sample was collected in each microenvironment so that the exposure concentration was known. The participant spent several hours in the microenvironment while the air sample was collected. Then the participant left the exposure area and immediately began providing breath samples. Breath samples were collected at multiple time points after the termination of exposure to develop a decay curve of breath VOC concentrations with enough time resolution to calculate a best fit linear function and clearance half-lives. Samples of air that the participant breathed during the 12 hours prior to entering the exposure environment and while providing breath samples after exposure were collected and analyzed to evaluate any confounding exposure to target VOCs outside of the selected microenvironment.

Most of the experiments were conducted using the same sample collection conditions, but there were some differences. An outline of the intended exposure and sample collection pattern is presented in Table 4-6 for five of the six exposure environments. Alveolar breath samples were collected in these five experiments. The fast collection rate using the alveolar method allowed more samples to be collected shortly after exposure ended. This allowed more accurate decay curves to be developed, particularly

TABLE 4-6. EXPOSURE EXPERIMENT SAMPLE COLLECTION OUTLINE[a]

Activity	Collection Time
Collect air sample prior to entering exposure environment	12 h, prior to exposure
Provide breath sample prior to entering exposure environment	15 min prior to exposure
Enter exposure environment, collect air sample	2-4 h, during exposure
Leave exposure environment, provide breath samples:	
Alveolar breath	3, 8, 18, 28, 38, 53, 68, 98, 128, 173, 218 min after exposure
Whole breath[b]	10, 30, 48, 70, 104, 134, 178, 223 min after exposure
Collect air sample at breath collection site	0 to 240 min after exposure concurrent with breath collection

[a] For all exposure experiments except consumer product experiment.

[b] Whole breath collected during three experiments; furniture stripping shop, hardware store No. 1, home garage.

during the initial phase of clearance from the body. Whole breath samples were collected along with alveolar breath samples during three experiments (furniture stripping, hardware store No. 1, home garage) to allow comparisons using this previously employed method [1-7,9]. The consumer product exposure experiment was conducted somewhat differently than the other experiments. Tenax cartridges were used to collect both breath and air samples to measure limonene, α-pinene, and p-dichlorobenzene concentrations. Since it was thought that the p-dichlorobenzene decay rate was much slower than those of the more volatile target chemicals breath, samples were collected over a much longer time period. An outline for the consumer product sample collection scheme is presented in Table 4-7. For all exposure experiments, one breath sample was collected immediately before the participant entered the exposure environment. This sample was intended to measure baseline breath concentrations for comparison to the measured concentrations after exposure.

Specific sample collection conditions for each of the 10 participant exposure experiments are described in Table 4-8. Two people alternated as the exposure participants for the first six exposures. These two participants were exposed to the hardware store atmosphere on the same day at the same time during another experiment (HS2, HS3). Two different people served as the participants in another experiment in which they were exposed to hardware store atmosphere at the same time (HS4, HS5). A description of the participants and their approximate breathing rates using the alveolar spirometer is presented in Table 4-9. A small meal was eaten by each of the participants approximately 30 to 50 minutes before the end of the exposure period. One exception to eating during the exposure phase was the swimming pool study in which the exposure period was cut short because the pool managers were going to open the pool area to the outside air. This action would have drastically altered the exposure concentration so the exposure was terminated after 2.3 h instead of 4 h. The exposure time in the garage experiment was limited to 2.2 h because this time was considered realistic for the acti- vity and the temperature was very high (37°C) in the garage. Conditions and activities at each exposure experiment microenvironment will be described in more detail in Section 6.

TABLE 4-7. CONSUMER PRODUCT EXPOSURE EXPERIMENT SAMPLE COLLECTION OUTLINE

Activity	Collection Time
Collect air sample prior to entering exposure enviroment	12 h, prior to exposure
Provide breath sample prior to entering exposure environment	15 min prior to exposure
Enter exposure environment, collect air sample	4 h, during exposure
Leave exposure experiment, provide whole breath samples	3, 21, 38, 57, 75, 100, 130, 175, 219, 433 min after exposure and 18, 31, 50, 68 h after exposure
Collect air samples during breath collection time period. Samples collected at:	0 to 6 h after exposure 6 to 25 h after exposure 25 to 50 h after exposure 50 to 68 h after exposure

TABLE 4-8. EXPERIMENTAL CONDITIONS AND SAMPLES COLLLECTED DURING EXPOSURE EXPERIMENTS

Experiment:	Furniture Stripper Shop	Hardware Store	Swimming Pool
Experiment Code:	FS1	HS1	SP1
Participant:	1	2	2
Hours exposed:	3.4 h	3.7 h	2.3 h
Experiment date:	3/29/89	4/7/89	4/21/89
Sample Collection			
Alveolar Breath			
Sample Type	2-L Canister	2-L Canister	2-L Canister
Number collected	12	12	12
Number duplicates	0	1	1
Number blanks	1	1	1
Number controls	1	1	1
Whole Breath			
Sample type	6-L Canister	6-L Canister	Not Collected
Number collected	9	9	
Number duplicates	1	1	
Number blanks	1	1	
Number controls	1	1	
Air			
Sample type	6-L Canister	6-L Canister	6-L Canister
Number collected	3	3	3
Number duplicates	0	0	0
Number blanks	0	0	0
Number controls	0	0	0

(continued)

TABLE 4-8 (cont'd.)

Experiment:	Wood and Metal Shop	Consumer Products	Garage, Fuel Wood Stain
Experiment Code:	WS1	CP1	GS1
Participant:	1	2	1
Hours exposed:	4.0 h	5.2 h	2.2 h
Experiment date:	5/9/89	5/12/89	5/25/89
Sample Collection			
Alveolar Breath			
Sample type	6-L Canister	Not Collected	6-L Canister
Number collected	12		12
Number duplicates	0		0
Number blanks	1		1
Number controls	1		1
Whole Breath			
Sample type	Not Analyzed	Tenax	6-L Canister
Number collected		15	8
Number duplicates		14	1
Number blanks		4	1
Number controls		4	1
Air			
Sample type	6-L Canister	Tenax	6-L Canister
Number collected	3	6	3
Number duplicates	1	3	0
Number blanks	0	3	0
Number controls	0	3	0

(continued)

TABLE 4-8 (cont'd.)

Experiment:	Hardware Store	Hardware Store	Hardware Store	Hardware Store
Experiment code:	HS2	HS3	HS4	HS5
Participant:	2	1	3	4
Hours exposed:	3.7 h	3.7 h	3.9 h	3.9 h
Experiment date:	6/7/89	6/7/89	6/21/89	6/21/89
Sample Collection				
Alveolar Breath				
Sample Type	6-L Canister	6-L Canister	6-L Canister	6-L Canister
Number collected	12	12	12	12
Number duplicates	2	2	2	2
Number blanks	1	1	1	1
Number controls	1	1	1	1
Whole Breath				
Sample type	Not Collected	Not Collected	Not Collected	Not Collected
Number collected				
Number duplicates				
Number blanks				
Number controls				
Air				
Sample type	6-L Canister	6-L Canister	6-L Canister	6-L Canister
Number collected	1	3	3	2
Number duplicates	0	1	0	0
Number blanks	0	0	0	0
Number controls	0	0	0	0

TABLE 4-9. PARTICIPANT CHARACTERISTICS AND APPROXIMATE ALVEOLAR SPIROMETER BREATHING RATES

Participant Number	Sex	Age	Height	Weight	Alveolar Spirometer Breathing Rate (breaths/min)
1	Male	35	178 cm	82 kg	4.8
2	Male	31	168 cm	57 kg	5.2
3	Male	32	185 cm	79 kg	5.6
4	Female	25	180 cm	61 kg	8.0

Exposure Experiment Sample Collection

Several sample types were collected during the exposure experiments including canister alveolar breath, canister whole breath, Tenax whole breath, canister air, and Tenax air samples. The Summa® polished stainless steel canisters were cleaned prior to sample collection by evacuation to 50 mtorr while being heated to 140°C for at least four hours in an oven (Figure 4-2). Canisters were stored under vacuum and the pressure differential was used to pull air and breath samples into the canister. Tenax GC was purified by extensive Soxhlet extraction in methanol and pentane followed by thermal desorption at 255°C under a purge of cryogenically cleaned helium. Tenax cartridges were stored in glass culture tubes inside a can in a solvent-free room before sample collection and in the tubes and can inside a freezer at -20°C after sample collection.

Two spirometer systems were used to collect breath samples during this study. The older spirometer, which has been used in many previous studies, collects the entire portion of exhaled breath expired over a period of 3 to 6 minutes, until a 40 L Tedlar bag is filled. Then the whole mixed breath contained in the bag is pulled into canisters or across a Tenax sorbent bed to trap the analytes. In contrast, the modified spirometer is designed to collect primarily alveolar breath into canisters while the participant is breathing into the device. Collection of whole breath samples requires 15 to 20 minutes while the new device allows sample collection times as short as two minutes.

Alveolar breath samples were collected using a modified spirometer system developed during the initial stages of this research project (Figure 4-3). Descriptions of the work performed to develop the alveolar spirometers are presented in Appendices A and B. Appendix A describes the initial feasibility study and Appendix B describes how, based on the results of the current work, the alveolar spirometer was made portable and characterized further. Briefly, the Tedlar bag used to store clean inhale air was rinsed with helium several times before each exposure experiment and was stored full of helium until collection of the first breath sample. The Teflon and stainless steel mouthpieces were steam sterilized prior to use. Immediately prior to collection of the first breath sample, the helium was expelled from the bag and the mouthpiece was installed on the van-mounted spirometer. The participant inhaled humidified ultrapure air

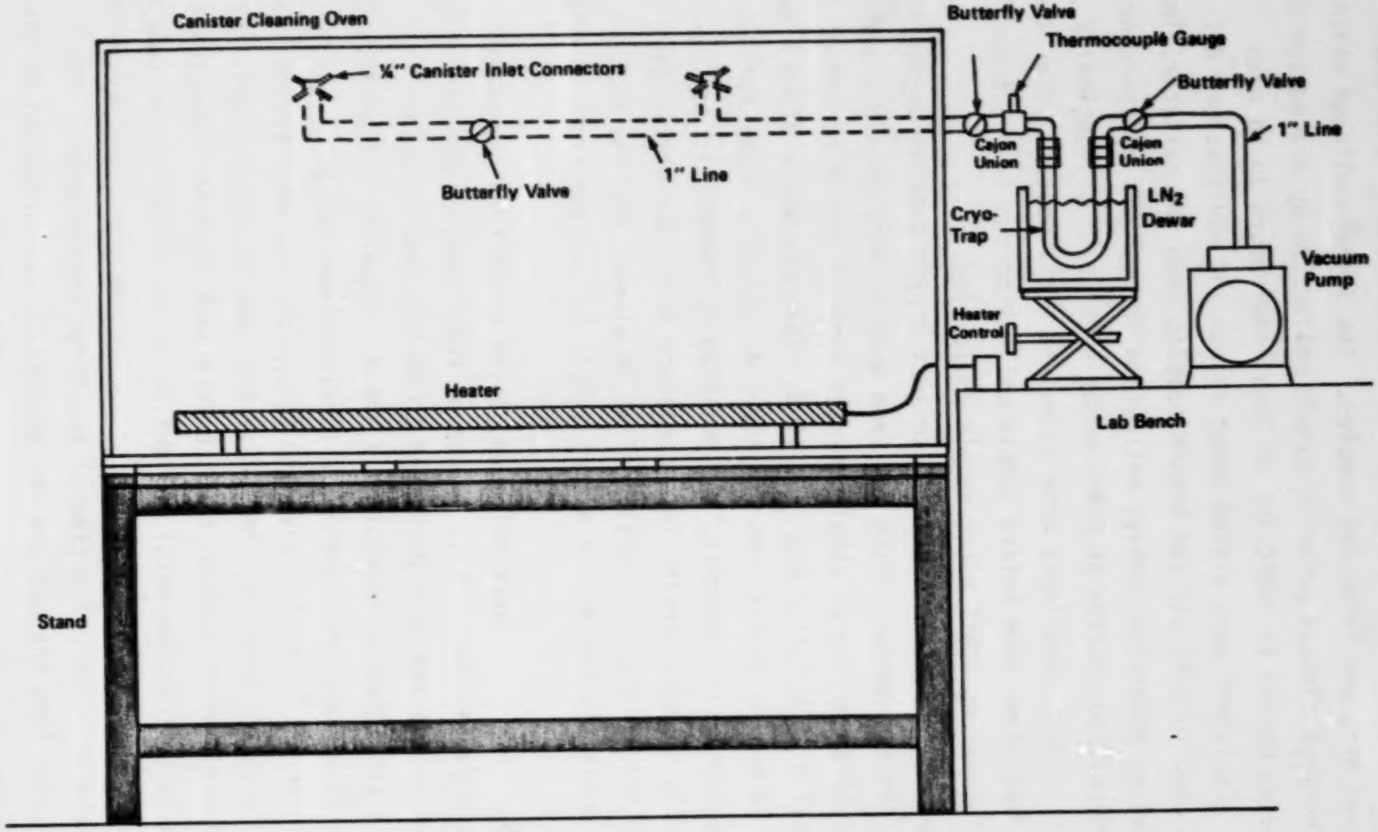
Canister Cleaning Oven
¼" Canister Inlet Connectors
Butterfly Valve
1" Line
Butterfly Valve
Thermocouple Gauge
Butterfly Valve
1" Line
Cajon Union
Cajon Union
Cryo-Trap
LN$_2$ Dewar
Vacuum Pump
Heater Control
Heater
Lab Bench
Stand

Figure 4-2. Canister cleaning system diagram.

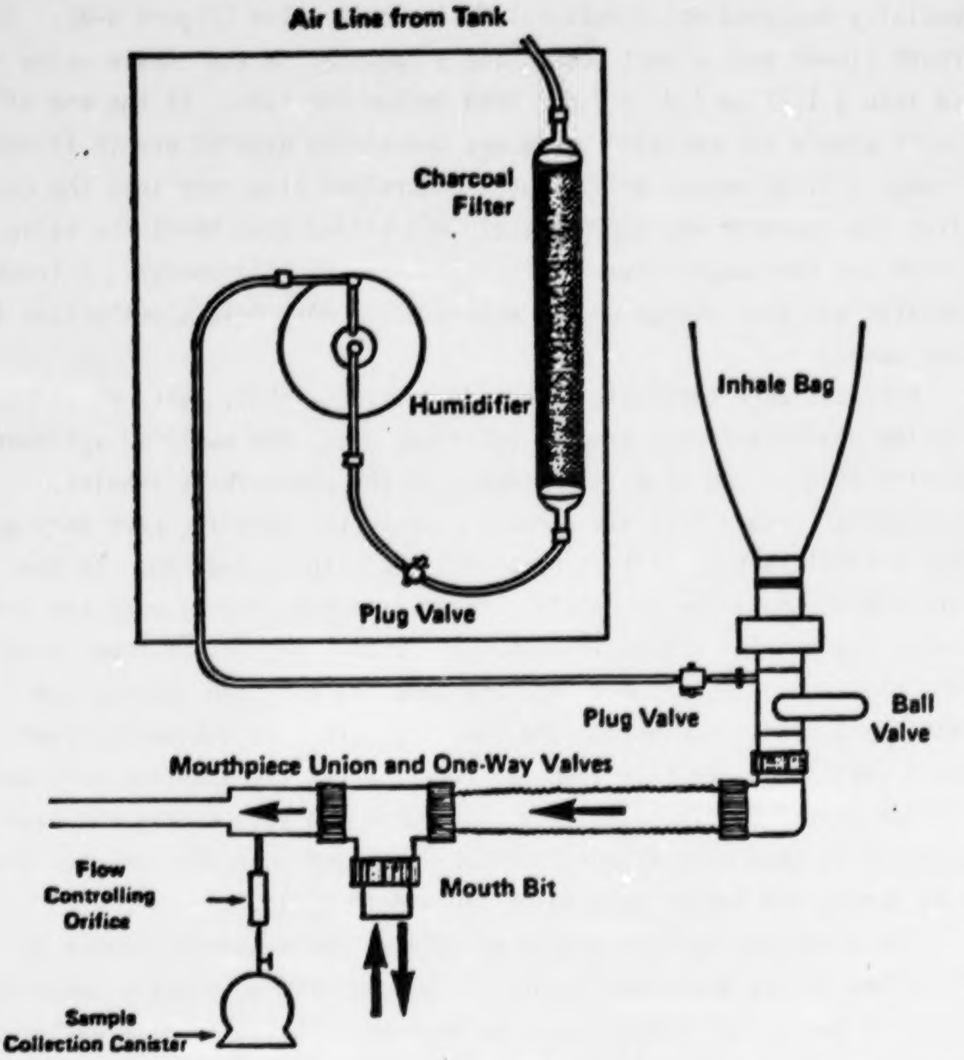
Air Line from Tank
Charcoal Filter
Humidifier
Plug Valve
Inhale Bag
Plug Valve
Ball Valve
Mouthpiece Union and One-Way Valves
Flow Controlling Orifice
Mouth Bit
Sample Collection Canister

Figure 4-3. Schematic diagram of the prototype alveolar spirometer system.

from the bag through one unidirectional valve and exhaled through a second specially designed unidirectional Teflon ball valve (Figure 4-4). The breath flowed past a port connecting a canister to the exhale valve exhaust and into a 1.27 cm i.d. x 7.6 m long Teflon FEP tube. At the end of the fourth exhale the canister valve was opened and exhaled breath flowed through a fixed needle orifice at a controlled flow rate into the canister. After the canister was approximately 80% filled (610 torr) the valve was closed and the subject ceased breathing into the spirometer. A fresh canister was then placed on the exhale valve port before collection the next sample.

Previous work (Appendix A) has demonstrated that, based on carbon dioxide concentrations, samples collected using the modified spirometer consist of over 97% alveolar breath. As the participant exhales, nonalveolar breath from his airways pass by the sampling port very quickly. Only a small portion of this nonalveolar breath is sampled. As the participant continues to exhale, breath from his alveoli pass the sampling port. The exhaled breath is contained in the long Teflon tube, with the nonalveolar breath farthest from the sampling port and end-expired (alveolar) breath closest to the sampling port. As the participant inhales the breath is pulled back down the tube towards the sampling port and into the canister. Sample collection flow rates and tube dimensions have been selected so that only alveolar breath is pulled into the canister from the tube during the inhale portion of the breath cycle.

The procedure for collection of VOCs in whole exhaled breath is described in the analytical protocol [9] and will be briefly summarized here. A Teflon and polyethylene mouthpiece with Tedlar flap valves and stainless steel ball valves was used (Figure 4-5). A gas impimger filled with distilled deionized water was placed in-line with the air tank to humidify the air for subject comfort. Each Tenax cartridge was connected to a separate Nutech 221 gas sampling pump so that the amount of air drawn through each cartridge could be accurately measured with the dry gas meter in the Model 221 pump. The inlet to the Tenax cartridge was connected to the Tedlar exhale bag using a 6 mm o.d. Teflon tube. Canister samplers were connected to flow controlling orifices placed in the Teflon tube between the exhale bag and Tenax cartridges. Breath samples were collected in evacuated canisters by opening the canister valves for a specified time

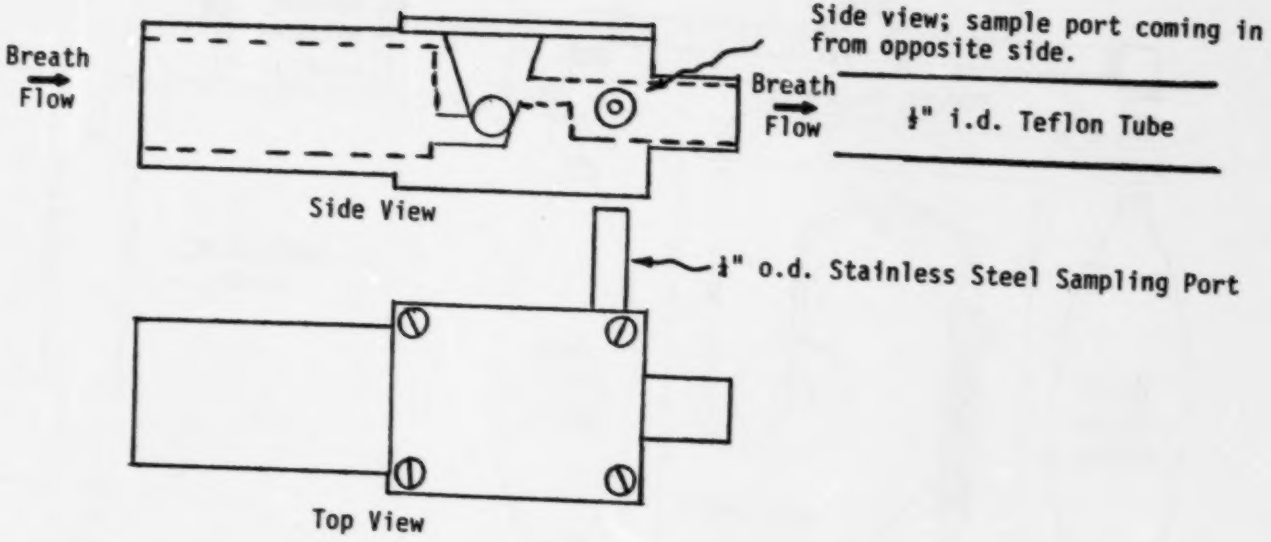
Breath
Flow
Side view; sample port coming in from opposite side.
Breath
Flow
½" i.d. Teflon Tube
Side View
¼" o.d. Stainless Steel Sampling Port
Top View

Figure 4-4. Exhale valve and sample port.

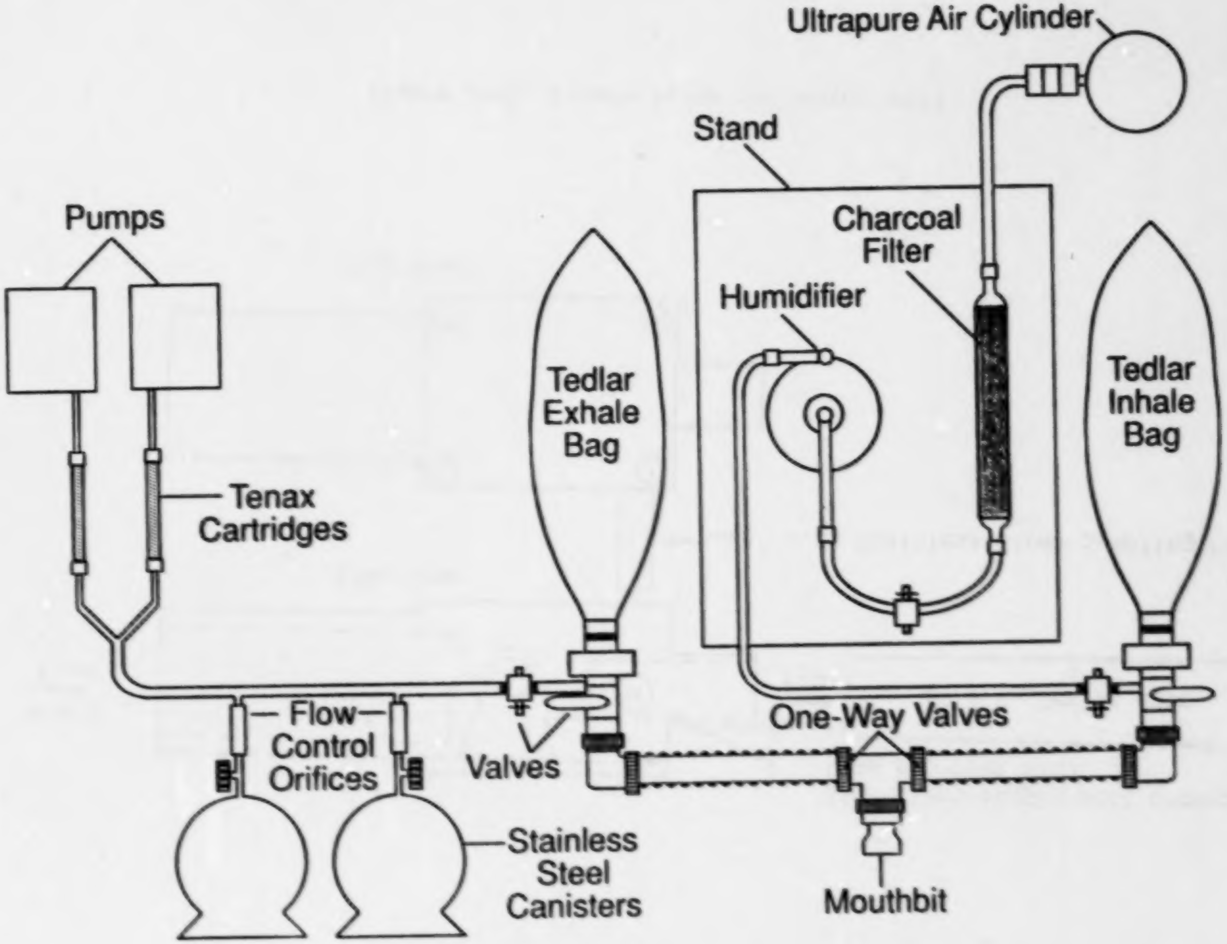
Ultrapure Air Cylinder
Stand
Pumps
Charcoal Filter
Humidifier
Tedlar Exhale Bag
Tedlar Inhale Bag
Tenax Cartridges
Flow Control Orifices
Valves
One-Way Valves
Stainless Steel Canisters
Mouthbit

Figure 4-5. Schematic diagram of the whole breath spirometer system.

period; the volume of exhaled breath collected in the canisters did not have to be accurately determined.

Immediately prior to the subject being seated at the spirometer, the inhale bag was installed and filled with approximately 40 L of purified, humidified air. A new piece of cleaned polyethylene tubing was used to connect the mouthpiece union to the elbow unions. The subject was seated on a stool and the mouthpiece height adjusted to a comfortable level. The subject was asked to wear nose clips and to inhale/exhale through the mouthpiece only. The Teflon plug was replaced with a sterilized Teflon mouthbit, the ball valves were opened and the participant began to breathe into the apparatus. When the sample bag was full, the subject was asked to stop breathing and the ball valves were closed. The Tenax cartridges were placed in line with the pumps and one or two canisters were connected to flow controlling orifices. The plug valve to the pump was opened and the sample is withdrawn from the bag through the cartridges. Approximately two minutes after beginning the sample flow through the Tenax cartridges the canister valves were opened. Exhaled whole breath was collected passively in the evacuated canisters due to the differential in pressure. The canisters were closed after 4.5 L of exhaled breath was collected in each; the amount of time open depended upon the size of the flow controlling orifice. Collection on the Tenax cartridges continued until the exhale bag was empty; approximately 15 to 16 L of exhaled breath was sampled on each of two Tenax cartridges.

After Tenax samples were collected, the cartridges were placed in culture tubes containing ca. 5 g of $CaSO_4$ and stored in sealed paint cans for 24 hours to dry the samples. The $CaSO_4$ was removed after 24 hours and the Tenax cartridges were placed in a freezer as soon as possible. The mouthbit was removed and replaced with the solid Teflon plug. The used collection bag (exhale bag) and polyethylene tubing were removed from the spirometer and replaced with clean materials before collection of the next sample.

Air samples were collected in canisters over 4-h periods in the exposure environment and in the van while breath samples were collected. Samples were collected over 12-h periods from the participant's air space during the period immediately prior to entering the exposure environment. Sample collection was initiated by attaching a flow controlling orifice to the canister and then opening the canister valve. A 4-h orifice was constructed for 6-L canisters by inserting three pieces of fused silica capillary tubing, each 60 µm i.d. x 25 mm long, through septum material in stainless steel tubing. The 12-h orifice used one piece of the fused silica capillary tubing. Each orifice was tested to ensure that a 4.5 L sample would be collected in each canister over the desired time period. Air samples collected in canisters using fixed orifices were slightly time weighted. The flow rate remained nearly constant until the canister was half-full (3 L) and then declined 15% to 20% as it approached three-quarters full (4.5 L). The air sampling canisters could not be worn due to their large size. The participant carried the canisters by hand whenever he/she moved.

The procedure for collecting VOCs in air using Tenax cartridges was described previously in this section for screening samples; this method was also applicable to collection of air samples during the exposure experiments. Personal air samples were collected by attaching the pump to the belt and the head of the cartridge to the collar in the breathing zone.

Blood samples were not collected and analyzed during these exposure experiments. The methodology developed for measuring low concentrations of VOCs in blood [10] was not suitable for conducting accurate decay measurements without modifications [7]. In an earlier phase of this research, attempts were made to improve the sensitivity of the blood method using alternative mass spectrometry procedures [11]. The goal of that research was to decrease the blood sample volume needed to measure exposures. A smaller sample size was mandatory because many samples needed to be collected over a short time period to accurately describe the elimination kinetics. The desired improvement in sensitivity was not achieved so blood samples were not collected.

SAMPLE ANALYSIS

Canister Analysis

The canister samples from air and breath were analyzed similarly. Because of differences in the mass spectrometer response due to different carbon dioxide and/or humidity levels, there were 3 separate calibrations for quantitative analysis. Alveolar breath calibration standards were prepared at 100% relative humidity and 4.8% CO_2, whole breath standards were prepared at 100% relative humidity and 3.8% CO_2, while air standards were prepared at about 25% relative humidity with no CO_2. In addition, the nominal sample volumes were 60, 80 and 200 mL for alveolar breath, whole breath and air samples, respectively, due to cryogenic trap freezing considerations. Each calibration consisted of a zero concentration level and 3 nonzero levels (ranging from 1.5 to 140 $\mu g/m^3$ for air and from 11 to 400 $\mu g/m^3$ for breath) appropriate for the concentrations expected. A point-to-point calibration was used in each case.

All samples and standards were analyzed by drying the air or breath through a Perma-Pure® dryer, then trapping a known volume in a cryo-cooled (-150°C) trap (Figure 4-6). An additional volume of d_6-benzene, perfluorotoluene and perfluorobenzene was also trapped separately to act as external standards. The trap was ballistically heated to transfer the trapped vapor onto a DB-624 fused silica capillary column which was temperature programmed. The analytical parameters are contained in Table 4-10.

Screening samples were analyzed by electron impact ionization MS in full scan or multiple ion detection (MID) mode. In some cases, a lower sample volume was trapped when VOC levels were expected to be elevated beyond the linear range of the instrument.

The amounts of target VOCs were calculated using the response ratio of d_6-benzene to each of the analytes. The calculations for all compounds except dichloromethane were carried out using a multi-level point-to-point calibration. Each level of concentration was based on a single analysis of a standard. Each standard injection consisted of the target compounds at one of the three concentration levels plus the external standards. The analytes were introduced at low levels (0.4 - 2 ng), medium levels (2 - 11 ng) or high levels (12 - 44 ng) into the instrument while the level of d_6-benzene was held constant (1.86 ng). The relative response factor (RRF) was calculated for each calibration level from

$$RRF = \frac{A_T/\mu g_T}{A_{std}/\mu g_{std}}$$

where A_T = the integrated peak area of the target analyte,
A_{std} = the integrated peak area of the external standard, d_6-benzene,
μg_T = the micrograms of a target analyte analyzed from a standard mixture of known composition

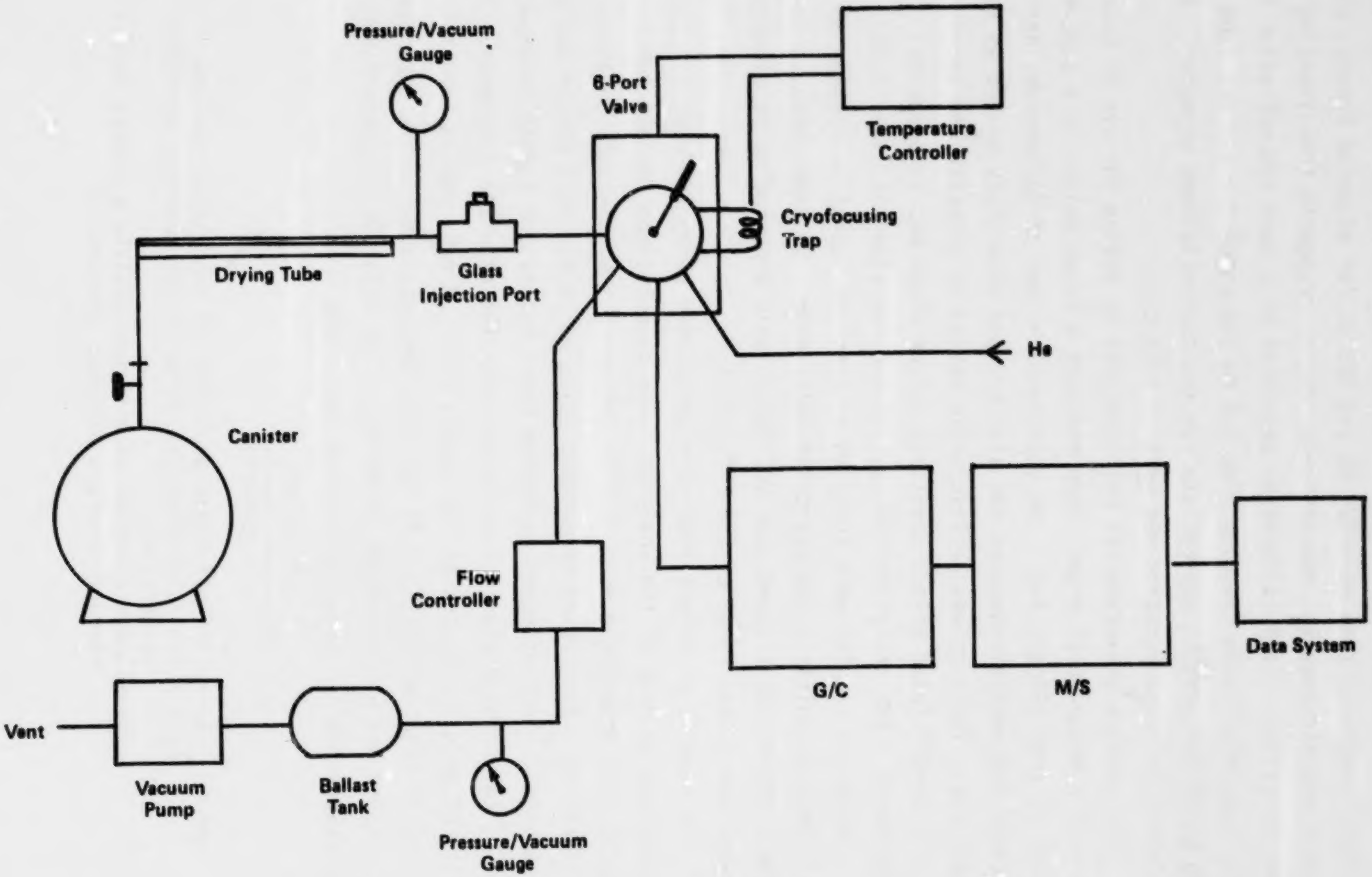
Pressure/Vacuum Gauge
6-Port Valve
Temperature Controller
Cryofocusing Trap
Drying Tube
Glass Injection Port
He
Canister
Flow Controller
G/C
M/S
Data System
Vent
Vacuum Pump
Ballast Tank
Pressure/Vacuum Gauge

Figure 4-6. Schematic diagram of the canister analysis system.

TABLE 4-10. ANALYTICAL CONDITIONS FOR CANISTER SAMPLE ANALYSIS

Instrument Component	Parameter	Setpoint or Condition
Canister interface	Temperature:	
	valve, 6-port	200°C
	transfer lines	200°C
	trap	-150°C → 200°C
	Sample Flow	20 sccm, nominal
	Trapping Time:	
	alveolar breath	3.0 min, nominal
	whole breath	4.0 min, nominal
	air	10.0 min, nominal
	external standard	2.5 min
	Dryer	Perma Pure, 1.1 m x 1/8" o.d.
	drying flow	80 mL/min nitrogen
Gas Chromatograph	Model	Varian 3700
	Temperature:	
	injector	200°C
	column	-20°C (0 min) @ 5°C/min → 200°C
	transfer line	200°C
	Column:	
	dimensions	30 m x 0.32 mm i.d.
	phase	DB-624
	Carrier gas:	Helium
	flow	~2.7 mL/min
	head pressure	10 psig (70 KPa)
Mass Spectrometer	Model	LKB 2091
	Type	magnetic sector, single focusing low resolution
	Operation modes	multiple ion detection (MID), full scan
	Ionization	electron ionization
	Ionization potential	70 eV
	Trap current	50 μA
	Multiplier:	
	preamplifier	1
	setpoint	500
	Temperature:	
	inlet	160°C
	source	180°C
	Full scan mode:	
	accelerating voltage	3.5 kV
	magnetic sweep range	1 → 256 *m/z*
	scan speed	1.5 sec/scan cycle

(continued)

TABLE 4-10 (cont'd.)

Instrument Component	Parameter	Setpoint or Condition
Mass spectrometer (continued)	MID mode:	
	magnetic setpoint	57 *m/z* @ 3.5 kV
	ions: min. and max.	57, 104 *m/z*
	scan speed, cycle	1 scan/sec
	Reference standard	tris-(heptafluoropropyl)-s-triazine
	Vacuum	2 x 10^{-5} torr
Data Acquisition	Computer	Tandy 3000 microcomputer
	MS interface and software	Teknivent Vector/1 system
	Sampling rate	10000 samples/sec
	MID mode:	
	sweep across ion	±0.2 *m/z* by 0.033 *m/z*
	sample time	1 mS
	samples averaged per ion	4 summed x 2 averagings
	A/D resolution	16 bit

μg_{std} = the micrograms of the external standard added to the analyzed standard aliquot.

By calculating the RRF for each calibration level, a point-to-point calibration could be constructed (RRF _vs_. the area ratio of the analyte to d_6-benzene). When a target compound was analyzed the area ratio ($area_{unk}/area_{ES}$) was used to determine the RRF from the curve. For levels below the low concentration level, the RRF of the low concentration standard is used. Once the RRF is determined, the amount (μg) can be calculated from

$$\mu g = \frac{A_T \times \mu g_{std}}{A_{std} \times RRF_{T/std}}$$

For dichloromethane, there often was splitting of the peak into two so the calculation was manually carried out on the sum of the areas using only a single RRF. This RRF was the average RRF of the three standards analyzed. The amount was calculated from the above equation.

Concentrations of several compounds that were not on the target list were estimated by using the response of similar target compounds. The compounds used are shown in Table 4-11. An average relative response factor (RRF) of the target compound across all concentrations was assumed to estimate the RRF of the nontarget compounds.

The garage experiment exposure air sample had analyte concentrations that resulted in signals that were far above the data system's range. This sample and one high level calibration standard were analyzed by full scan mass spectrometry at a reduced multiplier voltage. Analyte concentrations were estimated using a RRF based on the single calibration standard analysis.

A limit of detection (LOD) was determined for canister breath samples (Table 4-12). The LOD was calculated after the analysis of seven canisters fortified at very low concentrations of VOCs using 100% relative humidity and 4.8% CO_2. The LOD values were calculated using the equation:

$$LOD = S_r\ (t_{0.99})$$

where:

S_r = standard deviation of the response for replicate samples, in ng,

$t_{0.99}$ = Student's t value appropriate for a one-tailed test at the 99% confidence level and a standard deviation estimate with n-1 degrees of freedom

TABLE 4-11. ADDITIONAL COMPOUNDS AND THEIR QUANTITATION BASIS

Nontarget Compound	Target Compound with RRF Used
2-Methylhexane	n-Octane
3-Methylhexane	n-Octane
3-Methyloctane	n-Octane
n-Undecane	n-Decane
n-Dodecane	n-Decane
Ethylcyclohexane	2-Methylpentane
1,2,4-Trimethylbenzene	p-Xylene
Trimethylbenzene isomer	p-Xylene
n-Butyl acetate	1.2 x n-Octane[a]
2-Methylpropyl acetate	1.2 x n-Octane[a]

[a] Previous work on this instrument indicated a relative response factor 1.2 times that of octane for n-butyl acetate.

TABLE 4-12. LIMITS OF DETECTION AND QUANTIFIABLE LIMITS FOR CANISTER AND TENAX SAMPLE ANALYSIS

	Canister		Tenax	
Target Compound	LOD[a]	QL[b]	LOD	QL
		All values in ng		
Vinyl chloride	0.07	0.27	NT[c]	NT
Isopentane	0.06	0.25	NT	NT
Vinylidene chloride	0.03	0.13	NT	NT
n-Pentane	0.07	0.30	NT	NT
Dichloromethane	0.09	0.34	NT	NT
2-Methylpentane	0.08	0.32	NT	NT
Chloroform	0.03	0.10	NT	NT
1,1,1-Trichloroethane	0.17	0.66	NT	NT
Carbon tetrachloride	0.02	0.10	NT	NT
Benzene	0.06	0.24	NT	NT
Trichloroethylene	0.04	0.17	NT	NT
n-Octane	0.02	0.07	6	24
Toluene	0.02	0.08	NT	NT
n-Nonane	0.02	0.07	6	24
Tetrachloroethylene	0.09	0.36	NT	NT
Ethylbenzene	0.01	0.05	NT	NT
m,*p*-Xylene	0.01	0.04	7	28
Styrene	0.01	0.05	7	28
o-Xylene	0.02	0.09	7	28
α-Pinene	NT	NT	6	24
n-Decane	0.02	0.10	9	36
Limonene	NT	NT	7	29
p-Dichlorobenzene	NT	NT	18	72
n-Dodecane	NT	NT	9	36

[a] LOD = limit of detection.

[b] QL = quantifiable limit.

[c] Not a target compound.

A quantifiable limit (QL) was calculated as four times the LOD. The QL was used as the conservative cut-off point for concentration data to be included in curve fitting and half-life analyses of breath decay curves.

Canister Data Processing

The data from the GC/MS was put into an ASCII file format on a computer diskette. This included the compounds found and the amount detected. Irregularities in the data (e.g. incorrect peak assignment, etc.) were corrected by hand using a text editor. All corrected values were entered by hand into the ASCII report file.

Once the ASCII report file was corrected, the data was then imported into a Lotus Symphony spreadsheet. The spreadsheet was designed to automatically import data from each ASCII report file with minimal operator effort. Once all files for an experiment are imported, calculations are performed to verify that the measured VOC amount was equal or greater than the quantifiable limit. All concentration data were reported in concentration units of $\mu g/m^3$ corrected to 25°C.

Tenax Analysis

Exposed Tenax sample cartridges were analyzed by thermal desorption injection onto a capillary column gas chromatograph, followed by mass spectrometer detection. In brief, volatile organic analytes were thermally desorbed from the Tenax at 260°C with a nominal helium flow into a cryogenically cooled nickel capillary trap. The condensed vapors were then introduced into a high resolution fused silica capillary chromatography column by ballistic heating of the trap to 250°C. Mass spectrometer detection and characterization was performed using electron ionization with measurement of the intensity of the extracted ion current profiles. Typical operating parameters are described in Table 4-13. Relative response factors (RRF) were used to quantitate target compounds found during GC/MS analysis. The RRFs were generated by adding known amounts of an external quantitation standard, perfluorobenzene, to each calibration cartridge. The same amount of the external standard was loaded onto each sample cartridge. The amount of target analyte on each sample cartridge was calculated using the following equation:

TABLE 4-13. GC/MS TENAX ANALYSIS PARAMETERS

Parameter	Setting
Inlet-manifold	
Desorption chamber and valve	270°C
Capillary trap - minimum	-195°C
- maximum	240°C
Thermal desorption time	8 min
He purge flow	15 mL/min
GC	
Column	60 m DB1 wide bore fused silica
Temperature	40° (hold 5 min) - 240°C, 4°C/min
Carrier (He) flow	1.0 mL/min
Separator Oven	240°C
MS	Finnigan 4000
Scan range	m/z 35 → 350
Scan cycle, automatic	0.95 sec/cycle
Emission current	0.5 mA
Electron multiplier	1000 volts[a]
Hold time	0.05 sec

[a] Typical value.

$$\mu g_T = \frac{A_T \times \mu g_{std}}{A_{std} \times RRF_{T/std}}$$

where: A_T = integrated peak area of a target analyte
A_{std} = integrated peak area of a quantitation standard
μg_{std} = micrograms of quantitation standard added to the Tenax cartridge
$RRF_{T/std}$ = relative response factor of target analyte response to quantitation standard response

Since the volume of air collected for a sample was accurately known and the quantity of analyte per cartridge was determined, the breath concentration was calculated from:

$$\mu g/m^3 = \frac{\mu g_T \times 1000\ L/m^3}{\text{Volume sampled (L)}}$$

Calibration and daily response factor cartridges were prepared using flash evaporation techniques for all target compounds. The LODs and QLs for the target analytes were calculated as described above and are displayed in Table 4-12. Concentration values were not corrected for background amounts of the analytes or recovery of analytes from the Tenax cartridges. Background and recovery values are reported in Section 5.

SECTION 5
QUALITY ASSURANCE

ANALYTICAL PROTOCOLS

A Work Plan [12] and four Analytical Protocols [9] were prepared for this study. These protocols covered all study activities except alveolar breath sampling and analysis and are listed in Table 5-1. In addition, a Quality Assurance Project Plan (QAPP) [13] was prepared for this study to outline quality assurance (QA) and quality control (QC) objectives and procedures. Adherence to analytical protocols was not monitored during this study.

FIELD OPERATIONS/SAMPLE COLLECTION

Collection of screening samples was performed between January and June, 1989. Exposure experiment samples were collected between March and June, 1989.

Air and breath samples for screening and exposure experiments were collected in the Research Triangle Park area by two RTI chemists, each having over 10 years of Total Exposure Assessment Methodology (TEAM) field sampling experience. In addition, the Task Leader was present in the field during all exposure experiment sampling.

Samples were identified by sample codes generated for this study in the form:

140-EEE-MSTx

where the first three numbers identify the study. The next 3 letters (EEE) identify the experiment. The codes are:

SCR	Screening
FS1	Furniture stripping experiment
HS1	Hardware Store Experiments 1-5
HS2	
HS3	
HS4	
HS5	
WS1	Wood/Metal Shop Experiment
SP1	Swimming Pool Experiment
GS1	Garage/Stain Experiment
CP1	Consumer Product Experiment

TABLE 5-1. ANALYTICAL PROTOCOLS PREPARED FOR EXPOSURE ASSESSMENT STUDY

RTI/ACS - Protocol No.	Analytical Protocol Title
AP-202-004	Fixed-Site and Personal Monitoring of Vapor-Phase Organic Compounds in Ambient Air - Tenax
AP-203-008	Determination of Volatile Organic Compounds in Whole Blood
AP-203-007	Sampling and Analysis Procedure for Organics in Human Breath Samples
AP-203-003	Indoor and Outdoor Monitoring of Vapor-Phase Organics in Ambient Air - Canisters

The next three letters (MST) identify the sample type. Matrix type (M) codes are:

A	Alveolar Breath
W	Whole Breath
E	Air-Exposure Experiment
O	Overnight Air (before Exposure Experiment)
B	Air collected during breath collection

Sampling Device (S) codes are:

C	Canister
T	Tenax

Sample Type (T) codes are

F	Field Sample
D	Duplicate Sample
Q	Duplicate sample collected for analysis by the independent laboratory
FB	Field Blank
FC	Field Control

The last identifier is the sample sequence (x) number, usually 0-11.

A sample collection schedule was prepared at the start of the exposure experiment study. The schedule identified the times at which duplicate samples were to be collected and when field blanks and controls were to be utilized.

The study participants were RTI chemists. The exposure experiments were selected from potential activities and chemicals based on the results of the analysis of screening samples.

Projections for this study included collection of screening samples, and collection of air and breath samples immediately prior to, during, and after exposure to selected microenvironments. The exposure study sample projections were based on results of screening experiments and differ slightly from the numbers projected in the Work Plan (12). The completion rates for sample collection and analysis are shown in Table 5-2. A sample receipt report showing losses is shown in Table 5-3.

SAMPLE ANALYSIS

Screening Analysis

Screening samples collected on Tenax and in canisters were analyzed by capillary column gas chromatography/mass spectrometry/computer (GC/MS/-COMP) techniques. Full scan (FS) and multiple ion detection (MID) modes

TABLE 5-2. COMPLETENESS OF SAMPLE COLLECTION AND ANALYSIS

	Scheduled/Collected/Analyzed					
	Screening Samples		Exposure Experiment Samples[a]			
	Air		Breath		Air	
Sample Type	Canister	Tenax	Canister	Tenax	Canister	Tenax
Field Samples	32/32/32	9/9/9	144/144/134[b]	15/15/15	24/24/22[b]	6/6/6
Duplicate Samples	0/0/0	0/0/0	14/14/13[b]	10/10/10	3/3/3	1/1/1
QA Samples[c]	0/0/0	0/0/0	0/0/0	4/4/4	7/7/0	3/3/2
Field Blanks	0/0/0	0/0/0	12/12/12	4/4/4[d]	2/0/0	3/2/2
Field Controls	0/0/0	0/0/0	12/12/12	7/7/4[d]	2/0/0	3/2/2
Totals	32/32/32	9/9/9	182/182/171	37/37/37	37/34/25	16/16/14

[a] Numbers scheduled were based on results of analysis of screening samples.

[b] Explanation of sample losses given in Table 5-3.

[c] QA samples include performance evaluation samples and samples analyzed by an independent laboratory.

[d] One blank and one control analyzed by independent laboratory.

TABLE 5-3. SAMPLE RECEIPT REPORT

Sample Losses

1. Experiment SP1

   Sample 140-SP1-ACF11 had a leaky value, sample collected but not analyzed.

2. Experiments HS2 and HS3

   Sample 140-HS2-BCF1; canister was not opened; - not collected

3. Experiment WS1

   Whole breath samples not analyzed because only a few of the target compounds were found at levels sufficient for decay curves. Only alveolar samples analyzed for this experiment. Whole breath samples shifted to GS1 experiment.

4. Canister air sample blanks and controls

   There were not enough canisters to allow sample collection, breath blanks and controls and air blanks and controls.

5. Canister QA analysis

   - No independent laboratory was found for analysis of breath samples.
   - No independent laboratory was found that could analyze all target compounds at a reasonable price.
   - EPA supplied 3 canister air performance evaluation samples - these are the only canister QA samples.

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were used to determine, in a semiquantitative manner, the target compounds present. The results were used to select microenvironments for exposure experiments.

Exposure Experiment Samples

Tenax Samples--

Air and breath samples collected on Tenax were analyzed on a Finnigan 4021 quadrupole mass spectrometer on 8 analysis days between June 2 and June 14, 1989.

Prior to sample analysis, relative response factors (RRF) for each target compound were established by analyzing calibration cartridges prepared at 4 levels. Each cartridge also contained the quantitation standards perfluorobenzene (PFB) and perfluorotoluene (PFT). The levels of target compounds loaded onto Tenax cartridges for calibration are shown in Table 5-4. Based on the data from these analyses, average RRF values were calculated and used to quantitate the volatile organic levels in the samples.

A response factor cartridge was run at the beginning of each analysis day and agreement with the previously determined RRF values recorded. Each compound was considered in-control when the daily RRF was within ±30 of the mean calibration RRF.

The RRF values used for quantitation of volatile organic levels and the variability associated with the analyses are shown in Table 5-5. A summary of data from the daily response factor cartridges is shown in Table 5-6. Included for each analyte are the mean response factor (RRF) and the variability (%RSD) for the analysis period and the dates when the calculated daily RRF did not fall within the control limits. These results show that there were no instances when the daily response factors were outside the control limits.

In addition, the instrument tune was checked by measuring the intensity of PFT fragment ions relative to the base peak in the daily response factor cartridge. Control limits were based on ±20% of the mean values established during calibration (15 values). The PFT tune data acquired during sample analysis are shown in Table 5-7. The tune as measured by PFT relative ion abundances was within the acceptable range during the analysis period.

TABLE 5-4. LEVELS OF TARGET ANALYTES LOADED ONTO TENAX CARTRIDGES FOR CALIBRATION

Compound	Amount Loaded, ng/cartridge			
	1X	2X	4X	10X
n-Octane	211	422	844	2110
p-Xylene	260	520	1040	2600
Styrene	272	544	1088	2720
o-Xylene	260	520	1040	2600
n-Nonane	216	432	846	2160
α-Pinene	256	512	1024	2560
p-Dichlorobenzene	284	568	1136	2840
n-Decane	219	438	876	2190
Limonene	252	504	1008	2520
n-Dodecane	224	448	896	2240

TABLE 5-5. RELATIVE RESPONSE FACTORS USED FOR QUANTITATION OF VOLATILE ORGANICS IN TENAX SAMPLES

Compound	Ion	RRF	%RSD	N[a]
n-Octane	71	.47	7.7	8
	114	.12	5.3	8
p-Xylene	103	.10	4.7	8
	106	.86	5.3	8
Styrene	78	.63	4.7	8
	104	1.3	3.9	8
o-Xylene	91	1.6	4.8	8
	103	.10	6.8	8
	106	.76	6.1	8
n-Nonane	99	.11	5.7	8
	128	.10	6.3	8
α-Pinene	93	1.1	6.2	8
	121	.11	5.8	8
p-Dichlorobenzene	113	.18	6.4	8
	146	.92	6.5	8
	148	.62	7.0	8
	150	.11	11	8
n-Decane	99	.10	11	8
	142	.11	11	8
Limonene	68	1.0	8.5	8
	121	.13	7.1	8
	136	.17	6.7	8
n-Dodecane	85	.50	7.0	8
	170	.09	8.1	8

[a] Duplicate analyses of calibration cartridges at 1X, 2X, 4X, and 8X levels.

TABLE 5-6. RESULTS OF ANALYSES OF DAILY RESPONSE FACTOR TENAX CARTRIDGES

		RRF[a]		
Compound	m/z	Mean	%RSD	Out-of-Control Situations[b]
n-Decane	71	0.42	3.0	
	114	0.12	7.6	
p-Xylene	103	0.10	6.4	
	106	0.80	2.6	
Styrene	78	0.60	3.2	
	104	1.2	2.8	
o-Xylene	91	1.6	2.6	
	103	0.11	4.7	
	106	0.71	4.2	
n-Nonane	99	0.10	3.4	
	128	0.10	3.4	
α-Pinene	93	1.0	4.4	
	121	0.10	4.3	
	136	0.10	5.3	
p-Dichlorobenzene	113	0.16	4.2	
	146	0.84	2.2	
	148	0.57	3.2	
	150	0.09	4.6	
n-Decane	99	0.09	3.5	
	142	0.10	4.0	
Limonene	68	0.09	5.6	
	121	0.12	5.2	
	136	0.15	5.5	
n-Dodecane	85	0.45	2.8	
	170	0.08	4.0	

[a] Eight analysis days; mean of six values. No daily values for 6/2, 6/6/89.

[b] Daily value did not fall within control limits - ±30% of calibration RRF.

TABLE 5-7. PFT TUNE DATA, DAILY CHECK - FINNIGAN 4021

	PFT % Relative Abundance, m/z:							
Date:	69	79	93	117	167	186	217	236
6/2/89								
6/5/89	43.1	10.9	18.8	42.1	14.1	59.4	100	71.9
6/6/89								
6/7/89								
6/8/89	44.5	11.8	19.0	42.8	14.4	59.5	100	71.2
6/9/89	41.2	10.6	17.9	41.7	13.9	58.8	100	70.1
6/12/89	43.9	12.0	19.6	45.1	14.5	60.3	100	64.9
6/13/89	42.8	11.1	18.7	42.6	13.8	59.1	100	69.0
6/14/89	42.3	10.8	18.1	41.4	14.4	59.1	100	72.9
MEAN	43.0	11.2	18.7	42.6	14.2	59.4	100	70.0
SD	1.1	0.5	0.6	1.2	0.3	0.5	0.0	2.6
CV	2.5	4.6	3.0	2.8	1.9	0.8	0.0	3.7
Target Value[a]	43.7	11.4	19.0	42.3	14.2	59.1	100	70.9
Acceptable Range	35.0- 52.4	8.0- 14.8	13.3- 24.7	29.6- 55.0	9.9- 18.5	41.4- 76.8	-	49.6- 92.2

[a] Established 6-2/ - 6/5/89.

The performance of the sample inlet/chromatography system was checked before analysis of samples was begun and again near the end of sample analysis. Peak resolution (*o*-xylene and *n*-nonane) and separation number (*n*-octane and *n*-decane) were monitored. These values were acceptable for both determinations.

Canister Samples--

Three matrix types (whole breath, alveolar breath and air) collected in canisters were analyzed on an LKB 2091 GC/MS/COMP system on 43 analysis days between April 6 and July 5, 1989.

Prior to sample analysis, calibration was established for each target compound for each matrix type by analyzing calibration canisters. A minimum of three concentrations and a blank were analyzed to prepare each calibration. The calibration canisters were prepared using a canister loading system [9]; the blank was a canister filled with clean ("zero") air. Quantitation standards (d_6-benzene, perfluorobenzene, perfluorotoluene) were added to each analytical aliquot (standards and samples) during the cryofocussing step, prior to injection into the GC/MS/COMP system. The target compound levels used for calibration are shown in Table 5-8. A separate calibration series was prepared for each matrix type - whole breath, alveolar breath and air. Relative response factors (RRF) at each of the 4 points (zero air and 3 concentrations) were calculated using the d_6-benzene quantitation standard. The Teknivent software system utilized single RRFs at each level and interpolated on a point-to-point basis. This point-to-point calibration was then used to calculate the ng of each target compound in the samples analyzed. A new calibration was prepared when more than 3 analytes were out-of-control on an analysis day. The calibrations prepared were:

Matrix	Calibration Prepared	Analysis Days
Whole Breath	4/4 - 4/6/89	4/6 - 4/20/89
	6/2	6/2 - 6/5/89
Alveolar Breath	4/11/89	4/12 - 4/25/89
	4/26/89	4/26 - 6/1/89
	6/7 - 6/8/89	6/8 - 7/4/89
Air	4/14/89	4/14 - 4/17/89
	5/2/89	5/2 - 6/6/89
	6/16 - 6/18/89	6/16 - 7/5/89

TABLE 5-8. LEVELS OF STANDARDS USED TO PREPARE CANISTER SAMPLE CALIBRATIONS

	Alveolar Breath Levels ng/Aliquot Analyzed			Whole Breath Levels ng/Aliquot Analyzed			Air Levels ng/Aliquot Analyzed		
Compound	Low	Medium	High	Low	Medium	High	Low	Medium	High
Isopentane	0.67	2.16	10.7	2.16	4.70	18.8	0.36	2.36	11.8
Pentane	0.67	2.16	10.7	2.16	4.75	19.0	0.36	2.38	11.9
n-Octane	0.74	2.41	11.9	2.41	5.33	21.3	0.41	2.67	13.3
n-Nonane	0.74	2.41	11.9	2.41	5.45	21.8	0.42	2.73	13.6
n-Decane	0.78	2.53	12.5	2.53	5.54	22.2	0.42	2.78	13.8
Tetrachloroethylene	0.67	2.16	10.7	2.16	4.93	19.7	0.38	2.47	12.3
Trichloroethylene	0.94	3.05	15.1	3.05	6.66	26.7	0.51	3.34	16.7
Vinylidene chloride	0.78	2.53	12.5	2.53	5.52	22.1	0.42	2.77	13.8
1,1,1-Trichloroethane	0.86	2.80	13.9	2.80	6.09	24.4	0.46	3.08	15.2
Vinyl chloride	1.52	4.94	24.5	4.94	11.00	44.1	0.84	5.52	27.5
Toluene	0.74	2.41	11.9	2.41	5.26	21.0	0.40	2.64	13.2
2-Methylpentane	0.70	2.27	11.3	2.27	4.95	19.8	0.38	2.48	12.4
Benzene	0.74	2.41	11.9	2.41	5.30	21.2	0.40	2.66	13.3
Carbon tetrachloride	0.67	2.16	10.7	2.16	4.84	19.3	0.37	2.42	12.1
Chloroform	0.94	3.05	15.1	3.05	6.79	27.2	0.52	3.40	17.0
Dichloromethane	0.82	2.66	13.2	2.66	6.03	24.1	0.46	3.02	15.1
Ethylbenzene	0.74	2.41	11.9	2.41	5.26	21.0	0.40	2.64	13.2
p-Xylene	0.74	2.41	11.9	2.41	5.26	21.0	0.40	2.63	13.1
o-Xylene	0.74	2.41	11.9	2.41	5.27	21.1	0.40	2.64	13.2
Styrene	0.78	2.53	12.5	2.53	5.52	22.1	0.42	2.76	13.8

Levels for first calibration. Amounts varied slightly, depending on volume analyzed.

Quantitation standards approximately the same for all matrix types: PFB = 0.29 ng, PFT = 0.54 ng, d_6-Benzene = 1.87 ng.

A calibration standard (high level) was run once during each analysis day and the agreement with previously determined control limits recorded. The ng of each target compound calculated for this daily standard must be within ±30% of the known amount. Values more than ±30% from this known value were considered out-of-control. Corrective action was taken when more than 3 analytes were out-of-control on a given day. A summary of the daily checks for whole breath calibration is shown in Table 5-9, alveolar breath calibration in Table 5-10, and air calibration in Table 5-11.

In addition, the peak heights of the quantitation standards for each analysis were tabulated. This was to monitor the consistency of the GC/MS/COMP system. A summary of this QC check is shown in Table 5-12.

The performance of the sample inlet/chromatography system was checked June 2, 1989. Peak resolution (ethylbenzene and p-xylene) and separation number (n-octane and n-decane) were calculated. Both values were acceptable (resolution >1.0, separation number >40).

QC SAMPLE ANALYSIS (FIELD BLANKS AND CONTROLS)

Tenax Samples

The results of the analysis of Tenax field control samples are shown in Table 5-13. Three breath and two air controls were utilized. The results show consistently high recovery (87-98%) of all analytes. The data quality objectives [13] for recovery were met for all target compounds.

The results for the analyses of Tenax field blank samples are shown in Table 5-14. Four breath and two air blanks were utilized; no spirometer blanks were collected. The results show that the Tenax used for sampling was uniform and had very low background of target compounds.

Canister Samples

Blanks and controls were prepared for 2 of the 3 canister sample matrices - whole breath and alveolar breath. There were no blanks or controls for canister air samples. A QC set of one blank and one control canister was utilized for each breath matrix sampled during each exposure experiment. One alveolar breath blank and control were utilized for each exposure experiment; one whole breath blank and control were utilized during each of the three experiments where whole breath samples were collected. No spirometer blanks were collected during this study.

TABLE 5-9. DAILY CALIBRATION CHECKS - CANISTER WHOLE BREATH CALIBRATION APRIL 6 - APRIL 20, 1989, JUNE 2 - JUNE 5, 1989

Compound	m/z	Target Amount ng	Daily Check[a] Mean ng	%RSD	Out-of-Control Situations[b]
Isopentane	57	4.70	4.64	18	6/5
Pentane	57	4.75	4.82	16	
n-Octane[c]	57	5.33	4.91	18	
n-Nonane[c]	57	5.45	4.76	15	
n-Decane[c]	57	5.54	4.66	53[d]	4/11
Tetrachloroethylene	59	4.93	5.00	11	
Trichloroethylene	60	6.66	6.24	10	
Vinylidene chloride	61	5.52	5.29	10	
1,1,1-Trichloroethane	61	6.09	5.63	10	
Vinyl chloride	62	11.00	10.42	13	
Toluene[c]	62	5.26	4.91	10	
2-Methylpentane	71	4.95	4.47	15	
Benzene	78	5.30	5.00	11	
Carbon tetrachloride	82	4.84	4.55	7	
Chloroform	83	6.79	6.48	12	
Methylene chloride	84	6.03	5.42	7	
n-Octane	84	5.33	5.09	12	
n-Nonane	84	5.45	4.85	9	
n-Decane	84	5.54	5.96	7	
Toluene	91	5.26	4.84	9	
Ethylbenzene	91	5.26	4.98	8	
p-Xylene	91	5.26	4.64	12	
o-Xylene	91	5.27	5.05	6	
Styrene	104	5.52	5.07	10	

[a] Nine analysis days; mean of 5 values - no data for 4/7, 4/10, 4/20, 6/2/89.

[b] Results of daily check greater than ±30% of target amount. Corrective action not required if fewer than 3 target compounds are out-of-control on a given day.

[c] Two ions monitored for these compounds.

[d] Large %RSD due to a single value which may be an outlier.

TABLE 5-10. DAILY CALIBRATION CHECKS - CANISTER ALVEOLAR BREATH APRIL 12 - 25, 1989; APRIL 26 - JUNE 1, 1989; JUNE 8 - JULY 4, 1989

Compound	*m/z*	Target Amount ng	Daily Check[a]		Out-of-Control Situations[b]
			Mean ng	%RSD	
Isopentane	57	2.16	1.85	16	5/31
Pentane	57	2.16	1.85	17	4/21, 5/12, 5/15, 5/31
n-Octane[c]	57	2.41	2.12	17	6/22
n-Nonane[c]	57	2.41	2.15	14	6/22
n-Decane[c]	57	2.53	2.47	8	
Tetrachloroethylene	59	2.16	2.10	13	6/22
Trichloroethylene	60	3.05	2.98	10	
Vinylidene chloride	61	2.53	2.29	9	
1,1,1-Trichloroethane	61	2.80	2.66	9	
Vinyl chloride	62	4.94	4.49	12	
Toluene[c]	62	2.41	2.32	11	
2-Methylpentane	71	2.27	1.92	18	6/9, 6/12, 6/30
Benzene	78	2.41	2.09	16	5/31
Carbon tetrachloride	82	2.16	2.19	8	
Chloroform	83	3.05	2.87	9	
Methylene chloride	84	2.66	2.54[d]	14	6/26
n-Octane	84	2.41	2.26	25	6/22, 6/26
n-Nonane	84	2.41	2.29	20	6/22
n-Decane	84	2.53	2.35	14	6/30
Toluene	91	2.41	2.30	12	6/22
Ethylbenzene	91	2.41	2.33	12	6/22
p-Xylene	91	2.41	2.34	11	6/22
o-Xylene	91	2.41	2.33	10	6/22
Styrene	104	2.53	2.44	9	

[a] Twenty-nine analysis days; mean of twenty-three values. No data 4/12, 4/19, 4/25, 4/26, 5/9, 6/28/89.

[b] Results of daily check greater than ±30% of target amount. Corrective action not required if fewer than 3 target compounds are out-of-control on a given day.

[c] Two ions monitored for these compounds.

[d] N = 20.

TABLE 5-11. DAILY CALIBRATION CHECKS - CANISTER AIR
APRIL 14-17, 1989; MAY 2 - JUNE 6, 1989; JUNE 16 - JULY 5, 1989

Compound	*m*/*z*	Target Amount ng	Daily Check[a]		Out-of-Control Situations[b]
			Mean ng	%RSD	
Isopentane	57	11.8	11.5	17	
Pentane	57	11.9	11.3	15	
n-Octane[c]	57	13.3	13.1	17	
n-Nonane[c]	57	13.6	12.9	15	
n-Decane[c]	57	13.8	13.5	16	
Tetrachloroethylene	59	12.3	12.0	7	
Trichloroethylene	60	16.7	16.1	7	
Vinylidene chloride	61	13.8	13.4	12	
1,1,1-Trichloroethane	61	15.2	15.7	6	
Vinyl chloride	62	27.5	26.2	14	
Toluene[c]	62	13.2	12.4	11	
2-Methylpentane	71	12.4	11.9	16	
Benzene	78	13.3	11.8	13	
Carbon tetrachloride	82	12.1	11.8	4	
Chloroform	83	17.0	16.0	7	
Methylene chloride	84	15.1	14.0	6	
n-Octane	84	13.3	12.2	11	
n-Nonane	84	13.8	12.2	16	7/5
n-Decane	84	13.8	12.4	15	7/5
Toluene	91	13.2	12.0	10	
Ethylbenzene	91	13.2	11.9	10	
p-Xylene	91	13.1	12.1	13	
o-Xylene	91	13.2	12.0	9	
Styrene	104	13.8	12.3	9	

[a] Nine analysis days; mean of 5 values - no data for 4/14, 5/5, 5/10, 6/16/89.

[b] Results of daily check greater than ±30% of target amount. Corrective action not required if fewer than 3 target compounds are out-of-control on a given day.

[c] Two ions monitored for these compounds.

TABLE 5-12. SUMMARY OF EXTERNAL STANDARD PEAK HEIGHT MEASUREMENTS - LKB 2091 SYSTEM

Matrix	Dates	N	PFB Ave. Height[a]	PFB %RSD	PFT Ave. Height[a]	PFT %RSD	d_6-Benzene Ave. Height[b]	d_6-Benzene %RSD
Whole Breath Experiment 1	4/4-4/10/89	20[c]	591	14	1220	12	3970	18
Alveolar Breath Experiment 1	4/11-4/12/89	5[d]	580	11	1170	2.8	4070	12
Air, Experiment 1	4/13-4/17/89	19[e]	648	15	1260	12	4390	18
Air, Experiment 2	4/17/89	4	740	5.0	1490	11	5050	5.8
Whole Breath Experiment 2	4/18-4/20/89	18	577	6.5	1240	6.9	3980	7.9
Alveolar Breath Experiment 2	4/20-4/25/89	19	596	11	1210	4.1	4200	8.1
Alveolar Breath Experiment 3	4/25-4/27/89	27	728	5.6	1560	8.5	5220	9.9
LOD Determinations	5/1-5/2/89	9	676	3.6	1460	2.7	4620	7.6
Air, Experiment 3	5/2-5/3/89	7	908	6.1	1700	10	6290	7.0
Whole Breath Standards	5/4/89	4	743	2.2	1520	6.9	5450	1.6
Air, Experiment 4	4/9-5/10/89	7[f]	858	16	1630	12	6040	17
Alveolar Breath Experiment 4	5/10-5/15/89	16[g]	661	7.4	1490	6.7	4550	10
Alveolar Breath Experiment 5	5/26-5/31/89	26	685	11	1510	12	4590	12
Whole Breath Experiment 5	6/2-6/6/89	19[h]	575	28	1360	23	3590	22
Air, Experiment 5	6/6/89	3	836	12	1600	12	5650	16
Alveolar Breath Experiments HS2, HS3	6/6-6/14/89	42	512	16	1160	16	3010	10
Air, Experiments HS2, HS3	6/16-6/18/89	9	1002	10	1820	16	6940	10
Alveolar Breath HS4, HS5	6/22-7/5/89	49[i]	555	22	1190	16	2980	32

[a] Average peak height measured for *m/z* 69.

[b] Average peak height measured for *m/z* 84.

[c] 23 Analyses, data available for 20.

[d] 13 Analyses, data available for 5.

[e] 21 Analyses, data available for 19.

[f] 9 Analysis, data available for 7; includes 2 alveolar breath samples.

[g] 18 Analyses, data available for 16.

[h] 20 Analyses, data aveiable for 19.

[i] 50 Analyses, data available for 49.

TABLE 5-13. RESULTS OF ANALYSIS OF TENAX CONTROL SAMPLES

		Breath Controls				Air Controls		
		Amount Found, ng				Amount Found, ng		
	Amount Loaded ng	WTFC2	WTFC3	WTFC4	%REC[a] Mean	ETFC1	ETFC6	%REC Mean
n-Octane	211	195	179	184	88	194	173	87
p-Xylene	260	245	251	242	95	258	233	94
Styrene	272	277	270	255	98	276	252	97
o-Xylene	260	248	253	243	95	259	238	96
n-Nonane	216	198	205	194	92	210	193	93
α-Pinene	256	230	242	236	92	251	227	93
p-Dichlorobenzene	284	274	278	251	94	269	251	92
n-Decane	219	198	200	191	90	204	193	91
Limonene	252	231	229	231	91	241	220	91
n-Dodecane	224	205	200	196	89	202	186	87

[a] %REC = % Recovery.

TABLE 5-14. RESULTS OF ANALYSIS OF TENAX BLANK SAMPLES

	Breath Blanks[a]					Air Blanks[a]		
	Amount Found, ng					Amount Found, ng		
Compound	WTFB2	WTFB3	WTFB4	WTFB8	Mean	ETFB1	ETFB6	Mean
n-Octane	ND[b]	ND	2	2	ND	ND	2	2
p-Xylene	ND	ND	ND	ND	ND	ND	ND	ND
Styrene	7	ND	4	2	4	3	2	3
o-Xylene	ND	ND	ND	ND	ND	ND	ND	ND
n-Nonane	ND	ND	ND	ND	ND	ND	ND	ND
α-Pinene	ND	ND	2	ND	ND	2	ND	≤2
p-Dichlorobenzene	6	6	8	ND	6	5	ND	ND
n-Decane	ND	ND	ND	ND	ND	3	ND	≤3
Limonene	ND	ND	2	ND	ND	3	ND	≤3
n-Dodecane	ND	ND	2	ND	≤2	ND	ND	ND

[a] All reported values were at or below the quantifiable limit but above the LOD.

[b] ND = not detected.

Results of the analysis of control canisters are shown in Tables 5-15 (whole breath) and 5-16 (alveolar breath). The results for whole breath show good recovery for most compounds, between 80 and 98%. The data quality objectives for recovery [13], $\geq$80%, were met for all compounds except vinyl chloride, n-pentane, 2-methylpentane, n-nonane, and p-xylene. The variability (%RSD) was acceptable for most compounds. Higher variability for vinyl chloride, 2-methylpentane and tetrachloroethylene was due to one value being very different from the other two.

Results for alveolar breath controls show good recovery for most compounds, between 80 and 95%. The data quality objectives for recovery [13], $\geq$80%, were met for all compounds except 2-methylpentane and benzene. The results for n-pentane and dichloromethane are quite variable; all alveolar breath results for these compounds must be used with caution.

Results of the analysis of field blank canisters are shown in Tables 5-17 (whole breath) and 5-18 (alveolar breath). The results show very low background for all target compounds with one exception. Sample FS1-ACFB1 (alveolar breath blank, experiment FS1) showed measurable amounts of six target compounds.

DUPLICATE SAMPLE ANALYSIS

Tenax Samples

Seven duplicate pairs of samples were analyzed, one of the pair at RTI (F-type sample) and the other at the independent reference laboratory (D or Q-type sample). In addition, one control and one blank sample were analyzed by the independent laboratory. Only 3 target compounds were quantitated - α-pinene, limonene, and p-dichlorobenzene. The average percent relative standard deviation (%RSD) between sample pairs is shown in Table 5-19, and results of analysis of QC samples by the independent laboratory are shown in Table 5-20.

The amount of data is not sufficient to draw conclusions. A minimum of 2 blanks and 2 controls is recommended for each batch of samples analyzed by an independent laboratory and only one of each were analyzed for this study. Two pairs of air sample duplicates did not result in enough data to determine if data quality objectives were met [13] - $\leq$30% RSD. The results for analysis of breath samples all show %RSD values greater than the objective and greater than other recent data [5]. All of the values

TABLE 5-15. RESULTS OF ANALYSIS OF CANISTER WHOLE BREATH CONTROL SAMPLES

		Whole Breath Controls				
		% Recovery				
Compound	ng/L Loaded	FS1	HS1	GS1	Mean	%RSD[a]
Vinyl chloride	82.3	46	71	84	67	29
Isopentane	36.0	80	74	80	78	4
Vinylidene chloride	42.1	81	83	83	82	1
n-Pentane	36.0	77	79	62	73	13
Dichloromethane	44.4	83	104	99	95	12
2-Methylpentane	37.9	88	82	59	76	20
Chloroform	50.9	89	89	90	89	<1
1,1,1-Trichloroethane	46.7	88	87	86	87	1
Carbon tetrachloride	36.0	94	102	98	98	4
Benzene	40.2	85	77	84	82	5
Trichloroethylene	50.9	86	84	86	85	1
n-Octane	40.2	83	73	84	80	8
Toluene	40.2	82	87	87	85	3
n-Nonane	40.2	79	71	77	76	6
Tetrachloroethylene	36.0	84	84	113	94	18
Ethylbenzene	40.2	84	84	83	84	<1
p-Xylene	40.2	73	69	81	74	8
Styrene	42.1	85	83	82	83	2
o-Xylene	40.2	91	93	82	89	7
n-Decane	42.1	91	103	77	90	14

[a] %RSD = % Relative Standard Deviation.

TABLE 5-16. RESULTS OF ANALYSIS OF CANISTER ALVEOLAR BREATH CONTROL SAMPLES

		Alveolar Breath Controls										
		% Recovery										
Compound	ng/L Loaded	FS1	HS1	SP1	WS1	GS1	HS2	HS3	HS4	HS5	Mean	%RSD[a]
Vinyl chloride	82.3	70	96	85	90	75	99	79	86	82	85	11
Isopentane	36.0	67	83	82	78	64	93	78	89	83	80	11
Vinylidene chloride	42.1	80	92	82	81	76	98	85	88	85	85	7
n-Pentane	36.0	744	121	85	73	68	93	76	88	79	159[b]	131
Dichloromethane	44.4	331	86	99	101	106	90	89	111	114	125[c]	59
2-Methylpentane	37.9	62	91	87	64	58	75	78	72	71	73	14
Chloroform	50.9	75	94	92	92	83	99	89	90	88	89	7
1.1.1-Trichloroethane	46.7	58	87	87	94	79	105	90	101	91	88	15
Carbon tetrachloride	36.0	56	94	94	106	97	106	96	92	93	93	15
Benzene	40.2	61	88	87	79	59	96	80	84	80	79	14
Trichloroethylene	50.9	58	91	89	90	87	108	90	99	94	90	14
n-Octane	40.2	49	83	80	85	66	100	84	96	90	91	18
Toluene	40.2	62	95	88	86	75	97	85	89	83	84	12
n-Nonane	40.2	58	87	82	81	72	103	91	95	94	85	15
Tetrachloroethylene	36.0	70	92	94	97	90	95	90	95	91	90	8
Ethylbenzene	40.2	66	98	89	91	81	98	90	90	88	88	10
p-Xylene	40.2	72	98	89	95	85	99	92	92	90	90	8
Styrene	42.1	67	101	90	94	87	105	95	100	95	93	11
o-Xylene	40.2	66	98	89	93	85	98	93	94	90	90	10
n-Decane	42.1	84	102	86	85	89	101	94	113	111	96	11

[a] %RSD = % Relative standard deviation.

[b] Mean % Recovery (%RSD) without FS1 = 85(19).

[c] Mean % Recovery (%RSD) without FS1 = 100(10).

TABLE 5-17. RESULTS OF ANALYSIS OF CANISTER WHOLE BREATH BLANK SAMPLES

	Whole Breath Blanks Amount Found ng/L		
Compound	FS1 WCFB1	HS1 WCFB1	GS1 WCFB1
Vinyl chloride	ND[a]	ND	ND
Isopentane	ND	ND	ND
Vinylidene chloride	ND	ND	ND
_n_-Pentane	ND	ND	ND
Dichloromethane	ND	ND	ND
2-Methylpentane	ND	ND	ND
Chloroform	ND	ND	ND
1,1,1-Trichloroethane	ND	ND	ND
Carbon tetrachloride	ND	ND	ND
Benzene	0.8	1.0	0.7
Trichloroethylene	ND	ND	ND
_n_-Octane	ND	ND	ND
Toluene	ND	ND	ND
_n_-Nonane	ND	0.3	0.4
Tetrachloroethylene	ND	ND	ND
Ethylbenzene	ND	ND	ND
_p_-Xylene	ND	ND	ND
Styrene	ND	ND	ND
_o_-Xylene	ND	ND	ND
_n_-Decane	ND	0.1	0.3

[a] ND = not detected.

TABLE 5-18. RESULTS OF ANALYSIS OF CANISTER ALVEOLAR BREATH BLANK SAMPLES

	Alveolar Breath Blanks								
	Amount found, ng/L								
Compound	FS1 ACFB1	HS1 ACFB1	SP1 ACFB1	WS1 ACFB1	GS1 ACFB1	HS2 ACFB1	HS3 ACFB1	HS4 ACFB1	HF5 ACFB1
Vinyl chloride	ND[a]	ND	ND	ND	ND	ND	ND	ND	ND
Isopentane	ND	ND	ND	ND	ND	ND	ND	ND	ND
Vinylidene chloride	ND	ND	ND	ND	ND	ND	ND	ND	ND
n-Pentane	ND	ND	ND	ND	ND	ND	ND	ND	ND
Dichloromethane	ND	ND	ND	ND	ND	ND	ND	ND	ND
2-Methylpentane	ND	ND	ND	ND	ND	ND	ND	ND	ND
Chloroform	ND	ND	ND	ND	ND	ND	ND	ND	ND
1,1,1-Trichloroethane	ND	ND	ND	ND	ND	ND	1.0	ND	ND
Carbon tetrachloride	ND	ND	ND	ND	ND	ND	ND	ND	ND
Benzene	5.4	3.1	1.2	0.8	0.7	0.3	0.7	ND	0.7
Trichloroethylene	ND	ND	ND	ND	ND	ND	ND	ND	ND
n-Octane	ND	ND	ND	ND	0.5	ND	ND	ND	ND
Toluene	0.5	ND	0.3	ND	ND	ND	ND	ND	1.2
n-Nonane	ND	0.2	ND	0.2	0.5	ND	ND	ND	1.7
Tetrachloroethylene	15.6	3.4	ND	ND	ND	ND	ND	ND	ND
Ethylbenzene	1.5	0.3	ND	ND	ND	ND	ND	ND	ND
p-Xylene	5.9	0.7	ND	ND	ND	ND	ND	ND	ND
Styrene	ND	ND	ND	ND	ND	ND	ND	ND	ND
o-Xylene	2.9	0.5	ND	ND	ND	ND	ND	ND	ND
n-Decane	0.2	0.2	0.3	0.3	0.5	ND	ND	ND	ND

[a] ND = not detected.

TABLE 5-19. PERCENT RELATIVE STANDARD DEVIATION (%RSD) FOR DUPLICATE TENAX SAMPLES (INTERLABORATORY)[a]

	Breath Samples[b]		Air Samples	
Analyte	N[c]	Average %RSD	N	%RSD
α-Pinene	2	43	1	33
p-Dichlorobenzene	3	75	1	122
Limonene	4	60	1	60
Pairs Analyzed	4		2	

[a] Duplicate samples, one of the pair analyzed by the independent laboratory, the other by RTI.

[b] Whole breath samples.

[c] Number of pairs where both samples have measurable data.

TABLE 5-20. RESULTS OF ANALYSIS OF TENAX QUALITY CONTROL SAMPLES BY THE INDEPENDENT LABORATORY

	Blank	Control	
Analyte	ng Found	ng Loaded	% Recovery
α-Pinene	-[a]	256	57
p-Dichlorobenzene	18	284	57
Limonene	-	254	35

[a] Not found.

reported by the independent laboratory (including the control) are approximately half of the RTI values. Apparently there is a systematic error in the procedures used at one of the laboratories. It will be difficult to find the source of such an error since no standard reference materials are available and no performance evaluation samples were analyzed.

Additional duplicate sample pairs were collected and analyzed at RTI to obtain a measure of the variability of the sampling and sample handling procedures. The average %RSD between sample pairs is shown in Table 5-21. These data, though limited, show excellent intralaboratory precision.

Canister Samples

No canister samples were analyzed by an independent laboratory; no interlaboratory precision data are available. Intralaboratory precision was estimated by calculating the %RSD between duplicate pairs of samples analyzed at RTI. The average %RSD for duplicate canister samples is shown in Table 5-22. All of the values show good agreement, $\leq$30% RSD, except for several analyte/matrix combinations where there are only a single pair - n-octane in alveolar breath and chloroform in whole breath.

PERFORMANCE EVALUATION SAMPLE ANALYSIS

Three canisters, supplied by RTI, were fortified by AREAL/EPA-RTP. Each canister was given a legitimate study number and chain-of-custody form before being introduced into the sample analysis chain. The results were reported to EPA as ppb at reference conditions and without correcting for background and recovery. The results are shown in Table 5-23. The results show a high negative bias. No canister air matrix control samples were analyzed, so no % recovery results are available for comparison. All of the performance evaluation samples were run on a single analysis day (7/5/89). It appears likely that poor instrument performance, not detected by analysis of the daily calibration standard check, is the cause.

TABLE 5-21. PERCENT RELATIVE STANDARD DEVIATION (%RSD) FOR DUPLICATE TENAX SAMPLES (INTRALABORATORY)

Analyte	Breath Samples[a]			Air Samples	
	N[b]	Average %RSD	Range	N	%RSD
n-Octane	0	-	-	0	-
p-Xylene	1	3.8	-	0	-
Styrene	0	-	-	0	-
o-Xylene	0	-	-	0	-
n-Nonane	0	-	-	0	-
α-Pinene	7	5.0	0.0 - 12	1	3.5
p-Dichlorobenzene	10	2.6	0.4 - 6.9	1	9.1
n-Decane	0	-	-	0	-
Limonene	10	4.8	0.0 - 9.1	1	3.6
n-Dodecane	0	-	-	0	-
Pairs Analyzed	10			1	

[a] Whole breath.

[b] Number of pairs where both samples have measurable data.

TABLE 5-22. PERCENT RELATIVE STANDARD DEVIATION (%RSD) FOR DUPLICATE CANISTER SAMPLES (INTRALABORATORY)

Analyte	Alveolar Breath Samples		Whole Breath Samples		Air Samples	
	N[a]	Average %RSD	N	Average %RSD	N	Average %RSD
Vinyl chloride	0	-	0	-	0	-
Isopentane	6	6.2	2	7.1	2	5.2
Pentane	3	12.9	1	6.1	2	4.1
Vinylidene chloride	0	-	1	6.7	2	2.2
2-Methylpentane	1	7.1	1	1.9	2	2.7
Methylene chloride	9	3.4	2	2.8	2	5.1
Chloroform	5	10.7	1	44.8	1	3.8
1,1,1-Trichloroethane	9	3.6	1	4.2	2	2.4
Carbon tetrachloride	0	-	0	-	0	-
Benzene	0	-	1	0.0	1	0.0
Trichloroethylene	0	-	0	-	1	3.1
Toluene	10	5.2	3	2.5	2	3.6
n-Octane	1	31.8	1	18.9	2	1.2
Tetrachloroethylene	5	1.9	1	9.6	2	1.5
Ethylbenzene	6	10.9	2	3.4	2	1.0
p-Xylene	9	4.0	3	4.0	2	1.2
n-Nonane	8	6.5	2	4.3	2	4.6
Styrene	0	-	0	-	2	5.3
o-Xylene	3	7.1	2	2.9	2	1.7
n-Decane	7	12.8	1	1.5	2	11.9
Number analyzed	10		3		2	

[a] Number of pairs where both samples have measurable data.

TABLE 5-23. RESULTS OF ANALYSIS OF PERFORMANCE EVALUATION CANISTERS

Compound	Spiked, ppb		Reported, ppb[a]		% Bias[b]	
	No. 204	No. 206	No. 204	No. 206	No. 204	No. 206
Vinyl chloride	4.1	2.0	2.7	0.9	-34	-55
Dichloromethane	3.3	1.7	3.0	0.9	-9.1	-47
Chloroform	3.9	1.9	2.9	1.1	-26	-42
1,1,1-Trichloroethane	8.1	4.1	6.0	2.8	-26	-32
Carbon tetrachloride	3.8	1.9	4.0	1.8	5.3	-5.3
Benzene	4.2	2.1	2.4	0.6	-43	-71
Trichloroethylene	4.4	2.2	3.4	1.3	-23	-41
Toluene	8.2	4.1	5.6	1.6	-32	-61
Tetrachloroethylene	4.3	2.2	3.2	1.3	-26	-41
Ethylbenzene	7.5	3.7	4.9	1.5	-35	-59
o-Xylene	7.2	3.6	5.1	1.5	-29	-58

Sample No. 205 - zero air.

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[a] Reported at reference conditions.

[b] $\text{Bias} = \frac{\text{reported-spiked}}{\text{spiked}} \times 100.$

SECTION 6
RESULTS AND DATA ANALYSIS

INTRODUCTION

The primary goal of this research study was to increase our knowledge of the factors that affect the use of breath measurements as a tool for evaluating human exposure to VOCs. There were four principal objectives in this study, as described in Section 1. The first objective was to develop and test a canister based system for measuring VOC concentrations in alveolar breath. A system was developed and is described in Appendices A and B. This alveolar breath technique was employed to investigate elimination kinetics and was compared to a previously employed whole breath method. The second objective was to examine activities and microenvironments commonly encountered by the general population to determine the potential for exposure to VOCs. In this study the concentrations of 24 target compounds were measured in 32 microenvironments and in the headspace above six consumer products. A third objective was to determine breath VOC concentrations that resulted from exposure to a variety of chemicals in several microenvironments. Results are presented here for the breath concentrations before and at multiple time points after exposures in six micro-environments. The final objective was to calculate VOC residence times in the body, including half-life and best-fit curve functions. Breath decay half-lives were calculated using both a mono- and biexponential model. Several other mathematical curve-fit functions were evaluated for their fit against the experimental data.

SCREENING RESULTS

Introduction

Screening samples were collected in the air of 32 microenvironments and in the headspace above six consumer products. Target chemical concentrations were measured in each microenvironment screening sample. Results of the screening sample analyses were used to select several microenvironments for conducting exposure and breath elimination kinetics experiments. A primary goal of the microenvironmental screening was to find exposure scenarios for all target compounds that had concentrations high enough (typically >100 $\mu g/m^3$) for breath concentrations to be measurable for at least four hours after exiting the exposure location. A secondary goal of the screening was to provide a survey of microenvironments where a large portion of the population might be exposed to VOCs through short visits or under working conditions.

Three types of air samples were collected for screening purposes. Canisters were used to collect air samples in all 32 microenvironments and were analyzed for all target compounds except α-pinene and limonene. Air samples were collected on Tenax cartridges at 3 of the 32 locations in an effort to locate elevated concentrations of α-pinene and limonene. Headspace samples were collected over six consumer products using Tenax, also in an effort to locate a source of α-pinene and limonene that could be used in an exposure experiment.

Microenvironment Canister Screening Results

Air samples were collected using evacuated stainless steel canisters in 32 microenvironments that included homes, businesses, vehicles, and a swimming pool. All canisters were analyzed by GC/MS to determine the concentration of 22 target compounds including halogenated organics, aliphatic hydrocarbons and aromatic hydrocarbons. Most screening samples were collected as grab samples while several were collected over times ranging from 20 min to 12 h depending upon the exposure activity being characterized. Analytical results for the 32 microenvironment screening samples are presented in Table 6-1. Short descriptions of the conditions and results at each location are provided below.

Photocopier Room--

The copier room, located in a laboratory building, was a relatively small room with a Kodak copier. A small exhaust fan was in the room and the copier was in use for a short period just prior to air collection. The copier room was on the floor below organic and analytical chemistry labs. Low concentrations of several chlorinated compounds were observed as were very low levels of benzene and toluene.

TABLE 6-1. AIR CONCENTRATIONS ($\mu g/m^3$) IN MICROENVIRONMENT SCREENING CANISTER SAMPLES

Compound	Photocopier Room	Photocopy & Print Center	Oil-Based Painting	Metal Shop	Wood Shop	Wood Staining	Home No. 1 with Moth Crystals
Vinyl chloride	ND[a]	ND	ND	ND	ND	ND	ND
Isopentane	ND	ND	ND	ND	ND	ND	56
n-Pentane	ND	180	150	62	ND	1100	28
Vinylidene chloride	ND	ND	ND	4	ND	ND	ND
2-Methylpentane	2	2	ND	12	ND	58	1
Dichloromethane	20	10	25	23	5	2	3
Chloroform	7	50	77	36	ND	ND	14
1,1,1-Trichloroethane	2	5	3	21000	140	18	ND
Carbon tetrachloride	ND	ND	ND	ND	ND	ND	ND
Benzene	3	6	ND	ND	ND	10	8
Trichloroethylene	35	ND	5	8	15	5	ND
Toluene	8	9	20	130	120	2700	26
n-Octane	ND	ND	16	27	53	350	ND
Tetrachloroethylene	ND	ND	ND	1200	100	2	ND
Ethylbenzene	ND	1	24	4	90	11	7
m,*p*-Xylene	ND	5	88	11	200	30	13
n-Nonane	ND	2	230	26	8200	340	ND
o-Xylene	ND	4	39	4	75	11	9
Styrene	ND	ND	ND	ND	ND	2	ND
n-Decane	ND	ND	1200	63	1500	810	ND
p-Dichlorobenzene	ND	ND	ND	ND	ND	ND	22
n-Dodecane	ND	ND	46	NC[b]	NC	NC	NC

Compound	Home No. 2 With Moth Crystals	Office With One Smoker	Indoor Swimming Pool	Furniture Stripping Shop	Hardware Store No. 1	Hardware Store No. 2
Vinyl chloride	ND	ND	ND	ND	ND	ND
Isopentane	3	ND	24	10	29	630
n-Pentane	3	66	15	6	16	180
Vinylidene chloride	ND	ND	ND	3	2	ND
2-Methylpentane	3	ND	7	26	41	120
Dichloromethane	77	39	ND	7100	900	100
Chloroform	ND	36	240	2	ND	1
1,1,1-Trichloroethane	34	7	2	280	210	46
Carbon tetrachloride	ND	ND	ND	ND	ND	ND
Benzene	2	9	6	4	9	34
Trichloroethylene	ND	ND	ND	120	ND	6
Toluene	61	21	7	2500	650	250
n-Octane	1	ND	1	29	80	50
Tetrachloroethylene	ND	ND	ND	23	27	6
Ethylbenzene	47	1	3	120	590	17
m,*p*-Xylene	180	7	10	430	1700	64
n-Nonane	5	ND	2	61	290	200
o-Xylene	11	ND	4	160	110	23
Styrene	ND	ND	ND	68	38	7
n-Decane	9	ND	4	180	570	390
p-Dichlorobenzene	>540	ND	18	ND	39	ND
n-Dodecane	3	NC	ND	35	57	25

(continued)

TABLE 6-1 (cont'd.)

Compound	Interior Decorating Store No. 1	Interior Decorating Store No. 2	Beauty School No. 1	Beauty School No. 2	Laundromat	Bar/Club with Smokers	Rush Hour Driving With Smoking
Vinyl chloride	ND	ND	ND	ND	ND	ND	ND
Isopentane	35	9	21	43	11	74	61
n-Pentane	19	5	10	11	11	27	30
Vinylidene chloride	ND	ND	ND	ND	ND	ND	ND
2-Methylpentane	12	5	3	3	3	22	24
Dichloromethane	240	74	17	ND	6	6	5
Chloroform	ND	ND	20	6	36	6	2
1,1,1-Trichloroethane	22	12	72	8	2	3	5
Carbon tetrachloride	ND	ND	ND	ND	ND	ND	NC
Benzene	9	3	15	8	4	20	52
Trichloroethylene	ND	ND	12	7	ND	ND	ND
Toluene	310	27	240	320	6	54	120
n-Octane	21	53	2	ND	ND	2	3
Tetrachloroethylene	9	ND	ND	4	17	1	6
Ethylbenzene	28	7	5	2	1	10	23
m,*p*-Xylene	93	26	16	8	3	31	72
n-Nonane	380	190	6	3	ND	6	3
o-Xylene	22	11	5	2	1	13	23
Styrene	6	ND	7	ND	ND	6	17
n-Decane	700	590	14	2	ND	7	3
p-Dichlorobenzene	ND	90	3	3	2	NC	NC
n-Dodecane	NC	ND	6	2	ND	NC	NC

Compound	Truckstop Outdoors	Auto & Mower Refueling	Inside New Truck Cab	Home Garage A.M.	Home Garage P.M.	Commercial Repair Garage	Body & Repair Shop
Vinyl chloride	NC	1	ND	ND	ND	ND	ND
Isopentane	80	>1500	11	250	>370	79	88
n-Pentane	32	>3600	8	120	222	28	28
Vinylidene chloride	ND	1	1	ND	ND	ND	1
2-Methylpentane	18	>1900	15	62	110	19	23
Dichloromethane	ND	NC	7	2	1	4	4
Chloroform	ND	NC	2	1	1	ND	ND
1,1,1-Trichloroethane	1	2	160	3	2	1	68
Carbon tetrachloride	ND	NC	3	ND	3	ND	1
Benzene	8	>380	3	30	53	10	10
Trichloroethylene	ND	ND	1	ND	ND	ND	ND
Toluene	21	920	240	120	160	36	520
n-Octane	2	22	3	4	7	2	7
Tetrachloroethylene	ND	ND	2	ND	ND	ND	16
Ethylbenzene	5	110	27	26	32	7	56
m,*p*-Xylene	16	340	140	93	110	22	>210
n-Nonane	2	20	8	4	7	3	56
o-Xylene	6	120	68	32	40	10	71
Styrene	ND	13	33	6	10	ND	46
n-Decane	2	10	45	5	8	8	56
p-Dichlorobenzene	NC	NC	NC	NC	NC	NC	NC
n-Dodecane	NC	NC	NC	NC	NC	NC	NC

(continued)

TABLE 6-1 (cont'd.)

Compound	Paint & Body Shop	Home Diapers In Bleach	Mass Spec. Laboratory Facility	Laboratory with New Roof	Packaging Facility With Styrofoam
Vinyl chloride	ND	ND	NC	ND	ND
Isopentane	260	20	4	4	ND
n-Pentane	110	16	56	4	ND
Vinylidene chloride	ND	ND	ND	2	ND
2-Methylpentane	61	ND	9	2	ND
Dichloromethane	7	41	450	>1400	97
Chloroform	1	94	49	3	100
1,1,1-Trichloroethane	3	ND	13	53	ND
Carbon tetrachloride	ND	ND	1	ND	ND
Benzene	68	4	3	2	ND
Trichloroethylene	ND	ND	5	1	ND
Toluene	2100	11	180	3	14
n-Octane	35	ND	5	ND	ND
Tetrachloroethylene	ND	ND	1	ND	ND
Ethylbenzene	67	1	1	1	ND
m,*p*-Xylene	220	7	4	2	14
n-Nonane	36	2	1	2	ND
o-Xylene	80	2	1	1	ND
Styrene	19	2	1	ND	1
n-Decane	5	3	1	37	ND
p-Dichlorobenzene	NC	NC	NC	NC	NC
n-Dodecane	NC	NC	NC	NC	NC

[a] ND = not detected.

[b] NC = not calculated.

Photocopy and Print Center--

A high volume reproduction room was equipped with 3 Xerox copiers (in operation), an offset printer (off), and 4 binding machines. Chemicals in storage in this area were isopropyl alcohol, 1,1,1-trichloroethane, kerosene, 1,4-dioxane, butylene oxide, nitromethane, and styrene/acrylate polymer ink black. An outside door was open to the room and several exhaust fans were on. A photo processing lab was located in an adjacent room. Pentane and chloroform were found at moderately high concentrations at this location (180 and 50 $\mu g/m^3$) with all other target compounds present at ≤ 10 $\mu g/m^3$.

Oil-Based Painting--

A screening sample was collected from the air in an analytical laboratory in which the cabinets, doors, and trim were being painted with Glidden Wood Undercoater Oil Primer 310. Paint application began 1 h before the sample was collected. The normal building ventilation system was functioning and two doors leading to the hallway were open. Relatively high concentrations of some of the aliphatic hydrocarbons were measured as were somewhat lower levels of the aromatic hydrocarbons.

Metal Shop--

A metal shop, which was also adjacent to a woodworking shop, was sampled. The chemical products in use were a cutting fluid (1,1,1-trichloroethane), a degreasing solvent and, a safety coolant concentrate (including diethanolamine and monoethanolamine). The primary ventilation was from an open door and an open ceiling (in a larger building). Some machinery work had taken place prior to sampling. Very high 1,1,1-trichloroethane (21,000 $\mu g/m^3$) and tetrachloroethylene (1200 $\mu g/m^3$) concentrations were observed. These probably resulted from the cutting fluid in which the tetrachloroethylene may have been a minor component. Vinylidene chloride was found to be present as a trace component in the cutting fluid and was measured in the metal shop air at a concentration of 4 $\mu g/m^3$.

Woodworking Shop--

A woodworking shop, adjacent to the metal-working shop, had a light wood cutting schedule. Exhaust and recirculating (filtered) fans were on during cutting. Some wood glue was present but not in use. The main door to the shop was open to the rest of the building. Several target compounds were observed at concentrations above 50 $\mu g/m^3$ with n-nonane (8200 $\mu g/m^3$) and n-decane (1500 $\mu g/m^3$) the most prominant.

Wood Staining--

The wood staining air sample was collected in an area near the metal shop and the wood shop in the same building. The staining of recently constructed bookshelves had been completed just prior to the time of air sampling. The ventilation in this part of the building was relatively poor. High concentrations (>350 $\mu g/m^3$) of n-pentane, n-octane, n-decane, toluene were observed.

Moth Crystals; Home No. 1--

A bedroom, with mothballs in a closet, was sampled. The mothballs were p-dichlorobenzene and were in an open chest inside of a closet with the door kept closed. The bedroom was 10' x 12' and an interior room fan was on prior to air sampling. The p-dichlorobenzene concentration was relatively low at 22 $\mu g/m^3$ compared to concentrations measured in many homes during previous TEAM studies (1-5).

Moth Crystals; Home No. 2--

Two 4-oz moth crystals were located in a small closet in a den. The closet door was open while the den door was closed and there was no active ventilation. Results of the analysis of a screening sample collected in the den showed that p-dichlorobenzene was present at >540 $\mu g/m^3$ (the GC/MS signal was saturated during this analysis). It should be noted that the manufacturer recommended using four 4-oz moth crystals in a closet the size of the one in this house. Dichloromethane, toluene, and m,p-xylene were also present in this room and the source of these compounds was probably a sealed bottle of furniture refinishing solution stored in the closet.

Office with One Smoker--

A small office had one smoker who had smoked a cigarette prior to sampling. Several other cigarettes had been smoked earlier that same morning. The hallway door was open as well as a small exterior window. The office was located in a laboratory building, but was not directly connected to a laboratory. Only low concentrations (<10 $\mu g/m^3$) were observed for the tobacco combustion products benzene, ethylbenzene, m,p-xylene, and styrene.

Indoor Swimming Pool--

A screening sample was collected several feet above and away from the edge of an indoor swimming pool. The pool building's main ventilation system was not in operation and only one exhaust fan was blowing into an attached utility room. Chloroform was the target of this screening and was measured at a concentration of 240 $\mu g/m^3$. A block of deoderizer was found in an attached bathroom. It had the odor of p-dichlorobenzene which was present in the pool building air at a concentration of 18 $\mu g/m^3$.

Furniture Stripping Shop--

A furniture stripping/refinishing shop had furniture stripping operations underway prior to collection of the screening sample. Additionally, some carpentry was done and touch-up spray finish was used before or during air sampling. A number of pieces of furniture were sitting in the main area, presumably in the final stages of drying. The exterior doors were closed though there were exhaust fans on at the rear of the building. The furniture stripping solvent was primarily toluene and dichloromethane. Moderate to high air concentrations of many target compounds were observed.

Hardware Store No. 1--

A screening sample of air was collected in the center of the hardware store during business hours. The store stocked a wide variety of products including paints, paint removers, thinners, pesticides, home cleaning products, degreasing products, and bulk solvents as well as standard hardware and wood products. Most wood cutting and storage operations were performed in a separate building. A wide range of halogenated, aromatic, and aliphatic hydrocarbon target compounds was observed at concentrations ranging from 100 to 1700 $\mu g/m^3$.

Hardware Store No. 2--

This hardware store was very similar in terms of available products to the first store except fewer bulk solvents were sold at Store No. 2. The concentrations of halogenated and aromatic compounds were generally lower at this store while aliphatic hydrocarbons were at similar or higher levels.

Interior Decorating Store No. 1--

The interior redecorating store No. 1 contained primarily samples of vinyl flooring and rugs as well as various solvents and paints. A larger quantity of paints was stored in the rear of the building. Paint was mixed shortly before an air sample was collected. The solvents present included xylenes, toluene, paint stripper (dichloromethane), paint thinner, stains and oils. No obvious ventilation was noticed in the sales area. Many target compounds were observed in the screening sample, with levels above 200 $\mu g/m^3$ found for dichloromethane, toluene, n-nonane, and n-decane.

Interior Decorating Store No. 2--

The interior redecorating store No. 2 was similar to the previous one, though slightly smaller. Most of the target compounds measured in this screening location were at concentrations lower than the first store. Moderately high levels of n-nonane (190 $\mu g/m^3$) and n-decane (590 $\mu g/m^3$) were observed. The p-dichlorobenzene level (90 $\mu g/m^3$) was greater in this microenvironment than in any other except home No. 2 with moth crystals.

Beauty School No. 1--

The beauty school No. 1 had a low level of activity in a large room. A few permanents were being given at the time of sampling. Only a few hair products were visible, though more were probably stored in the cabinets. Ventilation, similar to that provided in most office buildings, was present. Many target compounds were observed at low levels while toluene was present at 240 $\mu g/m^3$.

Beauty School No. 2--

The beauty school No. 2 was similar to the first, though the activity for the size of the room was slightly greater. More hair products were on the shelf than at the first school. Once again, toluene was the only target compounds measured at an elevated concentration (320 $\mu g/m^3$).

Laundromat--

A screening sample was collected at a large, new, coin operated laundromat facility. Water used at this laundromat was supplied by a municipal water authority. Samples of this water supply have been analyzed in previous years and have contained chloroform levels ranging from approximately 50 ppb to above 100 ppb. During collection of the screening sample there were five washers and seven dryers in operation. Ceiling exhaust vents were in operation. A dry-cleaning operation was located within the same building next door to the laundramat. A door between the two was closed. The screening sample chloroform concentration was 36 $\mu g/m^3$.

Bar/Club with Smokers--

A small bar and nightclub facility was located in a basement area. The club was divided into two sections. The front section contained a bar, seating, and small stage. Several pool tables were located in the rear section. A short narrow hallway connected the two sections. The front section was nearly filled with approximately 45 patrons and the rear section contained approximately 15 patrons during sampling. Approximately 18-20 patrons were smoking cigarettes at the time of sample collection. One exhaust fan was operating in each section and a rear outside door was open. Benzene, toluene, xylenes, and styrene were observed at concentrations ranging from 6 to 54 $\mu g/m^3$.

Rush Hour Driving with Smoking--

An air sample was collected over a 75 minute period while the driver smoked 7 cigarettes and drove a crowded interstate and downtown loop route during morning rush hour traffic in Raleigh, NC. The car windows were closed and the ventilation system was set to the fresh air setting with a medium fan speed 30% of the time. The lighter aliphatic hydrocarbons and aromatic compounds were measured at concentrations ranging from 23 to 120 $\mu g/m^3$.

Truckstop, Outdoors--

A screening sample was collected outdoors at a large truckstop located at an interstate highway exit. The sample was collected about 20 m downwind from a row of 14 diesel and 2 gasoline pumps. Four diesel trucks, one small truck, and two cars were refueling during sample collection. The temperature was above 30°C at the time of sampling. Aliphatic and aromatic hydrocarbons were observed, with only isopentane (80 $\mu g/m^3$) and _n_-pentane (32 $\mu g/m^3$) at concentrations greater than 30 $\mu g/m^3$.

Auto and Mower Refueling--

A screening sample was collected over a 25 minute period during which time a car was driven to a gas station, the car fuel tank was filled, a 10 L fuel can was filled, the car was driven home, and fuel was added to a lawn mower. The fuel can was sealed and transported in the passenger compartment of the car in both directions. The air temperature was 25°C. The sample was collected near the breathing zone of the driver, who also did all fuel handling operations. Very high concentrations of the light aliphatic hydrocarbon (>1500 $\mu g/m^3$), toluene (920 $\mu g/m^3$), and benzene (>380 $\mu g/m^3$) were measured. Other target aromatic hydrocarbons were present at 110 to 340 $\mu g/m^3$.

Inside New Truck Cab--

An air sample was collected inside the cab of a new (<300 odometer miles) Chevy S-10 pickup truck to determine if a source of vinyl chloride could be found. The truck's dashboard, seats, and floor coverings were constructed from a plastic believed to be vinyl. The interior temperature was 42°C at the time of sampling. Vinyl chloride was not detected but moderately high levels of 1,1,1-trichloroethane, toluene, and m,p-xylene (140 to 240 $\mu g/m^3$) were observed.

Home Garage A.M. and P.M.--

The home garage was a 2-car detached garage that had some paint, paint thinner, gasoline, oil and kerosene stored in it. No appreciable ventilation was present. The P.M. sample was collected after a fully warmed up car was driven into it, the door was closed, and the engine turned off ~15 sec later. The air sample was collected 30 min later. The A.M. sample was collected before any activity occurred in the garage for the day, after the car had been parked overnight. Light aliphatic and aromatic hydrocarbons, consistent with fuel constituents, were observed in both samples. The concentrations were higher in the afternoon sample after the car was driven into the garage.

Commercial Repair Garage--

The repair garage was a bay-type repair garage with bays on each side of the building. Most bay doors were open. No other ventilation was present. Cars were inside all bays and active repair work was underway at the time of sample collection. All hydrocarbon concentrations were less than 100 μg/m^3. The concentrations measured under these highly ventilated conditions may be different in cooler weather when the bay doors are closed.

Body and Repair Shop--

The body and repair shop was a large building with approximately 10-12 cars inside. The building had its bay doors open and the building had some forced ventilation present. No automobiles were being painted and repair work in progress was relatively light. Toluene (520 μg/m^3) and m,p-xylene (>210 μg/m^3) were the most significant target compound concentrations measured at this microenvironment. Low levels of the aliphatic hydrocarbons (7 to 88 μg/m^3) were present. The highest microenvironmental styrene concentration (46 μg/m^3) was recorded at this location.

Paint and Body Shop--

The paint and body shop was a moderately sized shop with approximately 5 cars inside. No painting was going on at the time of collection. Two bay doors were open though no forced ventilation was present except for fans. A high toluene concentration was measured (2100 μg/m^3). Isopentane (260 μg/m^3) and m,p-xylene (220 μg/m^3) levels were observed as were lower concentrations of other aliphatic and aromatic hydrocarbons.

Home; Diapers in Bleach--

This sample was actually collected as one of the overnight 12-h samples prior to an exposure experiment. An unusually high chloroform concentration (94 μg/m^3) was observed in this sample. The home water supply came from a well and was not chlorinated, so it was unlikely that water was a source. No chloroform was observed in a similar sample from an earlier experiment. The only difference was the presence of soiled diapers soaking in a bleach solution in a closed pail in the bathroom. It was surmised, but not verified, that the soaking diapers was the source of the chloroform.

Mass Spectrometry Laboratory Facility--

A screening sample was collected in a laboratory facility containing five operating mass spectrometers in an effort to locate a source of the heavier aliphatic hydrocarbons for an exposure experiment. It was thought that the large number of vacuum pumps using oil might be an emission source. Only very low concentrations of these compounds were observed. Two common laboratory solvents, dichloromethane (450 $\mu g/m^3$) and toluene (180 $\mu g/m^3$), were observed.

Laboratory with New Roof Coating--

An opportunistic screening sample was collected after a new asphalt roof was applied to a laboratory building. Drums containing the asphalt material were stored directly below the air intake of a laboratory in which a very strong asphalt odor was observed. The screening sample showed only very low hydrocarbon concentrations. The dichloromethane (>1400 $\mu g/m^3$) resulted from extractions underway in the laboratory at the time of sample collection.

Packaging Facility with Styrofoam--

A screening sample was collected in a small room used for packaging materials for shipping. A large volume of styrofoam beads and shipping containers was stored in this room. This sample was collected in an attempt to find a source of styrene at levels high enough to conduct an exposure experiment. The measured styrene concentration was only 1 $\mu g/m^3$. The source of chloroform in this sample (100 $\mu g/m^3$) was not determined.

Nontarget Chemical Identifications

Nine of the screening samples were further examined to identify nontarget compounds present in significant amounts. Because this was a time consuming process, only nine samples were selected for qualitative analysis. Samples were selected based upon peaks observed in the original chromatographic traces. Results of this secondary data analysis are reported in Table 6-2. In most cases, aliphatic and aromatic hydrocarbons were identified along with an occasional fluorochlorocarbon or oxygenated compound. Dimethyl disulfide was tentatively identified in the swimming pool air. These identifications were not used for selecting exposure locations and were intended to provide general information on chemicals present in some microenvironments.

Compound identifications were made using a mass spectra library database. The spectrum of each unknown compound was compared to similar spectra in the library using a computer matching routine. A mathematical calculation was used to describe the degree of fit between the unknown compound spectra and the library spectra. The fit, measured as an R^2

TABLE 6-2. LIST OF NONTARGET COMPOUNDS PRESENT IN SELECTED SCREENING CANISTER SAMPLES

Furniture Stripper	Interior Decorating Store #1	Interior Decorating Store #2
trichlorofluoromethane	2-methyl-1,3-butadiene (tent.)	2-methylheptane
trimethylsilanol	3-methylhexane (tent.)	3-methylheptane
2-methyhexane	trimethylcyclohexane iso.	dimethylcyclohexane iso.
3-methylhexane	ethylcyclohexane	dimethylcyclohexane
acetic acid, 2-methylpropyl ester (tent.)[a]	trimethylcyclohexane	ethylcyclohexane (tent.)
ethylcyclohexane (tent.)	2-methyloctane	trimethylcyclohexane iso.
trimethylcyclohexane iso.[b]	3-methyloctane	2-methyloctane
3-methyloctane	methylethylcyclohexane	3-methyloctane
butanoic acid, 2-methylpropyl ester (tent.)	propylcyclohexane	ethylmethylcyclohexane
decane, branched chain (tent.)	4-cyclohexadecane (tent.)	alkylcyclohexane (tent.)
4-methylnonane		alkane, branched
1,2,4-trimethylbenzene (tent.)		*n*-undecane
1-ethyl-2-methylbenzene (tent.)		alkylcyclohexane
trimethylbenzene iso.		

Hardware Store #1	Hardware Store #2	Beauty School #1
1,2-pentadiene (tent.)	trichlorofluoromethane	trichlorofluoromethane
methylcyclopentane	pentene iso.	pentadiene
2-methylhexane	alkane (tent.)	2-ethylcyclobutanol (tent.)
3-methylhexane	alkane (tent.)	cyclic alkene or diene (tent.)
methylethylhexane (tent.)	hexane	*n*-undecane
ketone (tent.)	methylcyclohexane (tent.)	
2-methylheptane	dimethylpentane (tent.)	
3-methylheptane (tent.)	methylhexane	
acetic acid, 2-methylpropyl ester	branched alkane	
aldehyde or ketone (tent.)	branched alkane	
1,3,5-trimethylcyclohexane	alkyl cyclopentane (tent.)	
2-methyloctane (tent.)	branched alkane	
3-methyloctane	alkyl cyclohexane	
trans-1-ethyl-4-methylcyclohexane (tent.)	trimethylcyclohexane	
methylnonane iso. (tent.)	methyloctane iso.	
(1-methylethyl)-benzene	methyloctane iso.	
methylnonane iso. (tent.)	branched alkene iso.	
trimethylbenzene iso. (tent.)	alkyl cyclohexane	
1,3-cyclopentadiene,5-(1-methylpropylidene) (tent.)	alkane, branched	
ketone (tent.)	alkane, branched	
	alkane, branched	

Beauty School #2	Swimming Pool	Laundromat
With Perma Pure Dryer:		
trichlorofluoromethane	dimethyl disulfide (tent.)	ester (tent.)
pentadiene (tent.)		
decane, branched (tent.)		
decane, branched (tent.)		
undecane, branched (tent.)		
alkane, branched		
alkane, branched		
Without Perma-Pure Dryer:		
acetic acid, anhydride (tent.)		
acetic acid, butyl ester		

[a] tent. = Tentative GC/MS identification.
[b] iso. = Isomer.

value, generally had to be above 0.8 (on a scale from 0.0 to 1.0) for the tentative identification to be acceptable. One sample, from Beauty School No. 2, was analyzed both with and without the Perma-Pure dryer installed in the analytical system. The dryer was removed to determine if polar compounds were present in the sample. The drying tube prevents polar compounds from reaching the GC/MS system.

Microenvironment Tenax Screening Results

Air samples were collected on Tenax cartridges in three microenvironments in an attempt to locate a source of elevated α-pinene and limonene concentrations for an exposure experiment with those chemicals. The furniture stripping shop, hardware store, and woodshop were selected for screening since α-pinene was believed to be a natural wood emission product and because limonene was believed to be in wood finishing and care products used or sold at these locations. Each Tenax sample was collected over a 4 h period and was analyzed by GC/MS for 10 target compounds. The analytical results are reported in Table 6-3.

Most of the target compounds were found at measurable levels in each sample. Aliphatic and aromatic hydrocarbon concentrations were often above 100 $\mu g/m^3$ at all three locations with n-nonane and n-decane above 700 $\mu g/m^3$ in the wood shop and m,p-xylene above 600 $\mu g/m^3$ in the hardware store. Both α-pinene and limonene were found in all three locations but at relatively low concentrations. The highest α-pinene (34 $\mu g/m^3$) and limonene (12 $\mu g/m^3$) concentrations were measured at the woodshop. These concentrations were not believed to be sufficiently elevated to provide a measurable breath concentration several hours after an exposure. Since a suitable microenvironment for exposures to these compounds could not be identified, several consumer products were evaluated for α-pinene and limonene emissions.

Consumer Product Emissions Results

Six consumer products were tested including a pine oil, two furniture polishes, two room deoderizers, and one bathroom bowl cleaner. Samples were collected by a dynamic headspace purge onto Tenax cartridges followed by GC/MS analysis. Mass spectral data were examined for the presence of α-pinene and limonene plus any interfering components that could create problems during a later exposure experiment. There are many compounds

TABLE 6-3. AIR CONCENTRATIONS ($\mu g/m^3$) IN MICROENVIRONMENTAL SCREENING TENAX SAMPLES

Compound	Furniture Stripping Shop	Hardware Store No. 1	Wood Shop
n-Octane	26	29	110
m,p-Xylene	280	620	180
Styrene	35	15	3
o-Xylene	110	230	80
n-Nonane	71	110	730
α-Pinene	11	24	34
p-Dichlorobenzene	2	3	ND[a]
n-Decane	120	100	770
Limonene	2	5	12
n-Dodecane	25	1	68

[a] ND = not detected.

that are structurally similar to α-pinene and limonene that could have created data interpretation problems if present at significant quantities relative to the target compounds. Results of the qualitative analyses are presented in Table 6-4.

Both target compounds were observed in the Pine-Sol® samples, but there were also many other compounds present that had mass spectra similar enough to the targets to create interferences. The same result was also obtained for the Airwick® and Renuzit® room deoderizers. The Johnny Fresh® bathroom bowl cleaner emitted p-dichlorobenzene almost exclusively, with a small amount of a compound tentatively identified as α-fenchene that may have been responsible for the pine scent. Neither α-pinene or limonene were observed in the Old English® furniture polish. Both compounds were observed in the Wood Plus® furniture polish, and there were fewer potential interferents in this product than in the other products that were tested. Based on these results, Wood Plus® polish was chosen for use during an exposure experiment so that the breath levels of α-pinene and limonene could be examined.

Screening Results Discussion

The microenvironmental screening conducted during this research study was not intended as an exhaustive evaluation of all possible locations. Nor was it intended to define the range of concentrations that might be found across the country at all locations and under all conditions. At most, only one or two examples of each category were sampled at only one time point. Different results would undoubtedly be obtained for locations with different operating procedures, product lines, or ventilation conditions. For example, the auto repair garages were sampled in warm weather with the garage bays open. Higher concentrations of VOCs may have been measured in the winter with all bay doors closed. The screening results obtained during this study should not be extrapolated to represent all similar microenvironments. The results should instead be considered a snapshot at one time and place that might be an indicator of potential human exposure to volatile organic compounds.

The intent of screening microenvironments during this study was specifically to locate as many target compounds at the highest concentrations as possible. The screening results were evaluated and several

TABLE 6-4. QUALITATIVE RESULTS OF THE GC/MS ANALYSIS OF PRODUCT HEADSPACE SAMPLES FOR α-PINENE AND LIMONENE

Product Name	α-Pinene	Limonene	Potential Interfering Compounds
Pine-Sol® (19% pine oil)	Present	Present	Many
Airwick® Solid Room Deoderizer (lemon scent)	Present	Present	Many
Wood Plus® Polish (lemon scent)	Present	Present	Few
Johnny Fresh® Bathroom Bowl Cleaner (pine scent)	Absent	Absent	-[a]
Old English® Furniture Polish	Absent	Absent	-
Renuzit Roomate® Liquid Air Freshner	Present	Present	Many

[a] Not applicable since target compounds were absent.

microenvironments were selected as locations for conducting exposure experiments. Measurements of exhaled breath VOC levels were made after exposure to the microenvironment to evaluate whether such measurements can be a quantitative indicator of the original exposure.

EXPOSURE EXPERIMENT RESULTS

Introduction

Six microenvironments were selected for exposure experiments based upon the identities and amounts of VOCs in the screening samples. These locations included the furniture stripping shop, hardware store No. 1, the wood/metal shop, the indoor swimming pool, a home garage with wood staining and fuel handling, and a home with moth crystals and furniture polish. For each experiment, one participant was exposed to VOCs in the microenvironmental air for several hours. This participant provided one breath sample before, and multiple breath samples after the exposure. The goal was to determine the degree to which breath concentrations of each chemical were elevated by the exposure and the kinetics of elimination after the exposure. Air samples were collected within the microenvironment during each experiment to determine the VOC exposure levels. Air samples were also collected from the participant's airspace before and after each experiment to determine if they had unintended exposures to the target compounds.

The measured concentrations of organic compounds in each breath sample were studied in a number of ways. First, if the overnight air sample showed an insignificant exposure level when compared to the experimental exposure, and the pre-exposure breath concentration was low, then the measured breath levels were plotted as a function of post-exposure time. In this manner, qualitative information regarding the observed decays was acquired. Of special concern were the differences observed between decay curves for the same compound derived from whole breath and alveolar breath collections. Second, concentration/time data for each compound were subjected to a bivariate curve-fitting analysis to screen and study the ability of seven different mathematical functions to define the observed decay. Of particular interest was the ability of each equation to accurately predict a breath concentration for times throughout the entire range of collection times. Third, the data were fit to mono- and biexpontial (e^{-kt} and $e^{-k_1t} + e^{-k_2t}$) curves, corresponding to one and two physiological compartments, respectively, in an attempt to estimate the elimination half-life of each compound from the body and to study the effects of multiple compartment assumptions. Finally, these half-lives were examined for evidence of dependence on exposure level or the individual exposed.

Selection of Exposure Microenvironments

Six microenvironments were chosen for exposure experiments based on screening results. The screening samples were collected in two phases. The first phase included samples from the furniture stripping shop and hardware store No. 1. These two locations contained many of the target compounds at concentrations believed to be high enough for measuring breath decays over 4 h time period after exposure. Target compounds present at these two locations included halogenated organics, aromatics, and the less volatile aliphatic hydrocarbons. Breath decay data were collected successfully for many of the target compounds in these two microenvironments.

Chloroform was found at an indoor swimming pool at a concentration sufficiently high to allow breath decay measurements and an exposure experiment was successfully completed there. Screening samples from the wood/metal shop indicated large amounts of the less volatile aliphatic compounds might be found. However, the high concentrations were not observed during the exposure experiments. One surprising compound, vinylidene chloride, provided measurable breath concentrations after exposure in the wood/metal shop. This compound was found to be a trace component of the metal cutting fluid for which 1,1,1-trichloroethane was the primary constituent.

The second phase of the screening sample collection was used to try to locate sources of compounds not found in the first four experiments. These included benzene, styrene, vinyl chloride, carbon tetrachloride, the aliphatic hydrocarbons, α-pinene and limonene. Sources tested included smoking areas and vehicle related activities. One exposure experiment was conducted in a home garage which included fuel handling and wood staining. This experiment resulted in successful breath decay measurements for virtually every aromatic and aliphatic hydrocarbon except styrene. The last exposure experiment was conducted in a home with two consumer products, wood polish and moth crystals. Breath decay measurements were made for p-dichlorobenzene, limonene, and α-pinene in this microenvironment.

No sources suitable for decay studies were found for vinyl chloride, carbon tetrachloride, and styrene. Styrene was observed in several microenvironments, but always at concentrations lower than 45 $\mu g/m^3$, which was too low for breath decay measurements. No measurable concentrations of vinyl chloride were found in any microenvironment, including a new truck cab with copious amounts of vinyl maintained at a high temperature. No carbon tetrachloride levels above 3 $\mu g/m^3$ were measured in any screening samples.

Since exposure locations for three compounds (vinyl chloride, carbon tetrachloride, and styrene) could not be readily found, a decision was made to eliminate breath decay studies for these compounds. Repeat exposure experiments were performed at one location for several other compounds to provide some data for inter- and intraperson variability in breath levels and elimination kinetics. The hardware store was chosen for these repeat experiments because of the wide range of compounds measured successfully in the first experiment. In a second experiment, the two participants who had alternated exposures in the earlier experiments were both exposed to hardware store air at the same time. Both participants provided breath samples at the same time points after exposure using two separate alveolar spirometers. A final experiment was conducted in which two new participants were exposed to hardware store air and then provided breath samples during the same time period.

Description of Exposure Experiments

Furniture Stripper Shop--

Participant No. 1 was exposed to the air in a furniture stripping and refinishing shop for 3.5 h. Shop operations during the exposure period included dipping furniture into stripping vats, gluing, and a small amount of finishing. Chemicals known to be in use included toluene and dichloromethane in the stripping vats. Large exhaust fans were on at one end of the building while a small door was open at the other end. The participant provided both alveolar and whole breath samples over a 4 h period after exposure.

Hardware Store, First Exposure--

Participant No. 2 was exposed to the air inside a hardware store for 3.7 h. Several shelves were stocked with paints, thinners, degreasers, stripping agents, and bulk solvents. Pesticides and home cleaning products were also on sale at this store. No solvent handling or paint mixing was observed in the store during the exposure period. A ceiling mounted heater was blowing warm air down the aisle with paints and solvents toward the participant. The participant provided alveolar and whole breath samples over a 4 h period after exposure.

Indoor Swimming Pool--

Participant No. 2 was exposed to the air in an indoor swimming pool for 2.3 h. The exposure was scheduled for 4 h but was cut short when the manager decided to open a wall of exterior doors to increase the ventilation. This likely would have decreased the indoor chloroform concentration making data analysis more difficult. Very little ventilation occurred in the building during the exposure period. The participant sat approximately 3 m from the side of the pool and 1.5 m above the pool surface. A group of approximately 15 children were completing a swimming lesson as the exposure period started. A free swim period attended by 10 persons was the only activity during the exposure. The participant provided alveolar breath samples over a 4 h period after exposure. It should be noted that this participant was exposed to a relatively high time weighted average concentration of chloroform (94 $\mu g/m^3$) during the 12 h prior to the exposure experiment. It was surmised that diapers soaking in bleach in his home were the source of this exposure. The swimming pool air concentration was 600 $\mu g/m^3$, which was over five times higher than the overnight exposure. The first breath concentration after exposure was 81 $\mu g/m^3$, compared to 9 $\mu g/m^3$ before exposure.

Wood/Metal Shop--

Participant No. 1 was exposed to the air in a wood and metal shop for 4.0 h. Wood shop operations included sawing, sanding, and gluing. Metal shop operations were performed during the last hour of the exposure period and included metal cutting using a cutting fluid. The participant divided his time equally between the two adjacent shops during the last hour of exposure. Both alveolar and whole breath samples were collected over a 4 h period after exposure. Only the alveolar samples were analyzed since the less volatile aliphatic hydrocarbons were not found as expected.

Consumer Products--

Participant No. 2 was exposed to the air in one room of a house with moth crystals and furniture polish in use. Two four ounce p-dichlorobenzene moth crystals had been placed in the room two days prior to the experiment. An open container of Wood Plus® furniture polish was placed in the room. Every 40 minutes the polish was applied to both sides of a 0.2 x 0.9 m board with a rag. The participant wore gloves during each application to avoid dermal exposure. To avoid re-exposure, the participant changed clothes immediately before beginning the post-exposure breath sample collection. Breath samples were collected over a 68 h period after exposure since the half-life of p-dichlorobenzene elimination was expected to be much longer than that of most other target compounds [7]. Multiple air samples were collected in the participant's breathing zone over time after the exposure to determine if he was exposed to other sources of p-dichlorobenzene. The p-dichlorobenzene levels in these air samples decreased over time but were measurable even when the participant was at home, where the air sample prior to exposure showed very little p-dichlorobenzene. It was believed that the Tenax cartridge in the participant's breathing zone was adsorbing p-dichlorobenzene being exhaled by the participant.

Garage with Staining and Fuel Handling--

Participant No. 1 was exposed to emissions from automobiles, fuel handling, and wood staining operations during a 2.2 h period in a garage. The 2 car detached garage had very little ventilation and the temperature reached 37°C so the exposure period was reduced from 4 h. Several activities occurred during this exposure experiment. Two warm cars were driven into the garage and run 1 min. Stain was applied to 0.8 m^2 of plywood by someone other than the participant twice during the exposure period. Gasoline was transferred between a can and lawnmower four times and kerosene was also transferred between a nonfunctioning heater and can four times. All fuel was handled by someone other than the participant. The participant sat approximately 3 m from the staining and fuel handling operations. The participant changed clothes immediately before providing breath samples. Alveolar and whole breath samples were collected over a 4 h period after exposure.

Hardware Store, Second Exposure--

Participant Nos. 1 and 2 were exposed to air in the same hardware store at the same time for 3.7 h. The participants were seated approximately 2 m apart in the crowded store. The heating system was off and the air conditioning system was on; otherwise conditions were identical to those in the first hardware store exposure. The participants changed clothes immediately prior to collection of breath samples. Alveolar breath samples were collected at the same time from each participant using two spirometer systems over a 4 h period after exposure.

Hardware Store, Third Exposure--

Participants No. 3 and 4 were exposed to air in the same hardware store at the same time for 3.9 h. All conditions were the same as the second exposure in the hardware store. The participants changed clothes immediately prior to collection of breath samples. Alveolar breath samples were collected at the same time from each participant using two spirometer systems over a 4 h period after exposure.

Decay Data from the Exposure Experiments

In this section, the main observations regarding the types of compounds measured in the breath will be summarized for each exposure experiment. Complete information regarding the measured concentrations of organic compounds in breath for each experiment can be found in Appendix D. All of the air data for each experiment are included in Appendix D before the corresponding breath data. In addition, for those compounds that provided measurable concentrations in breath for seven or more collection periods, breath VOC data were plotted as a function of time after exposure ended. These plots are presented in Appendix E. The QL for the compound is given with each graph. Because the QL was dependent upon the volume of sample analyzed, it was not the same for every experiment or breath type. Any point that appears on a graph was above the QL for that particular analysis. Selected examples will be presented in the text along with appropriate comments.

Furniture Stripper Shop (Figures E-1 through E-4)--

The measurement of the organic compounds in the breath after exposure in the furniture stripper shop showed that four compounds were present in a sufficient number of samples to provide decay information. These compounds were dichloromethane, 1,1,1-trichloroethane, toluene, and m,p-xylene. Meta- and para-xylene are reported as one compound because they were not chromatographically resolved. Breath concentrations ranged from a high of 460 µg/m3 for toluene to 15 µg/m3 for m,p-xylene. Even at the relatively low levels measured for m,p-xylene, a decay was observed. For illustration, these decays are shown in Figure 6-1. The decay for toluene (Fig. 6-1A) is clearly defined. The short sampling times and higher collection frequency for the alveolar samples helped to define the very early phase of the decay curve. Although the measurements of the compound in whole breath provided a very good decay curve, rapid changes and possible subtle features in the curve were missed because of these samples. The longer time required to collect whole breath samples also restricted the number of data points that could be generated during the first few minutes after exposure ended. A more detailed discussion of the comparison of alveolar breath with whole breath appears later.

Figure 6-1B shows a clearly defined decay for m,p-xylene, even at levels near the QL. The alveolar values at 17 and 102 minutes are presumably the result of contamination of the 2 L canisters used here because this phenomenon was observed in another experiment that used the same canisters. In addition, these canisters had been used previously to collect samples with high levels of aromatic compounds. No such concentration deviations were observed in the whole breath samples. This potential contamination illustrates the importance of using clean canisters. The fact that we were measuring a series of concentrations and studying the kinetics made this contamination more evident.

Hardware Store, First Exposure (HS1, Figures E-5 through E-12)--

This experiment provided data for the elimination decays of dichloromethane, 1,1,1-trichloroethane, toluene, tetrachloroethylene, ethylbenzene, m,p-xylene, n-nonane, and o-xylene. This exposure situation resulted in moderate levels of at least two classes (chlorinated hydrocarbons and aromatic compounds) of chemicals. Deviations from the curves

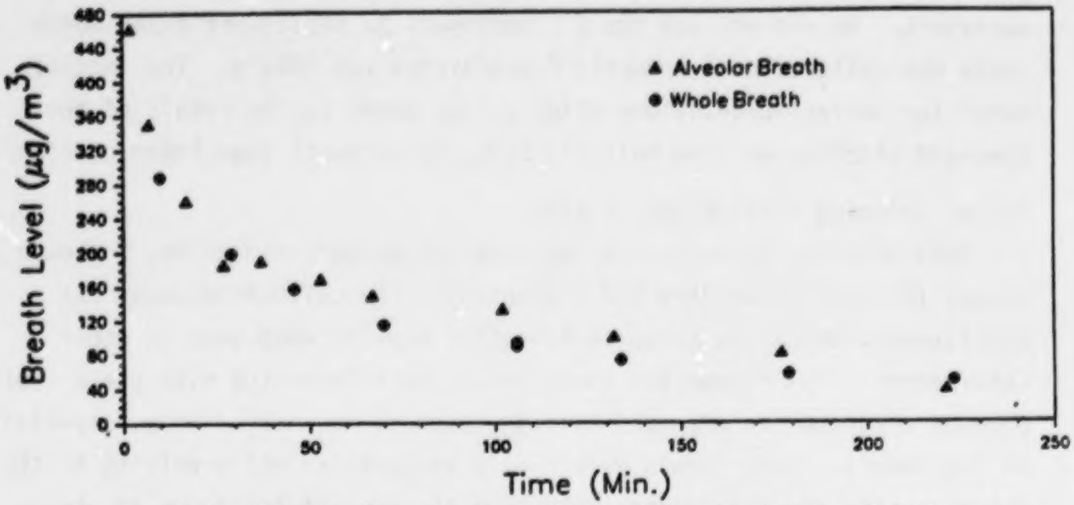

Figure 6-1A. Breath levels of toluene post-exposure to furniture stripping operations. Exposure: 5700 μg/m^3; QL = 6 μg/m^3.

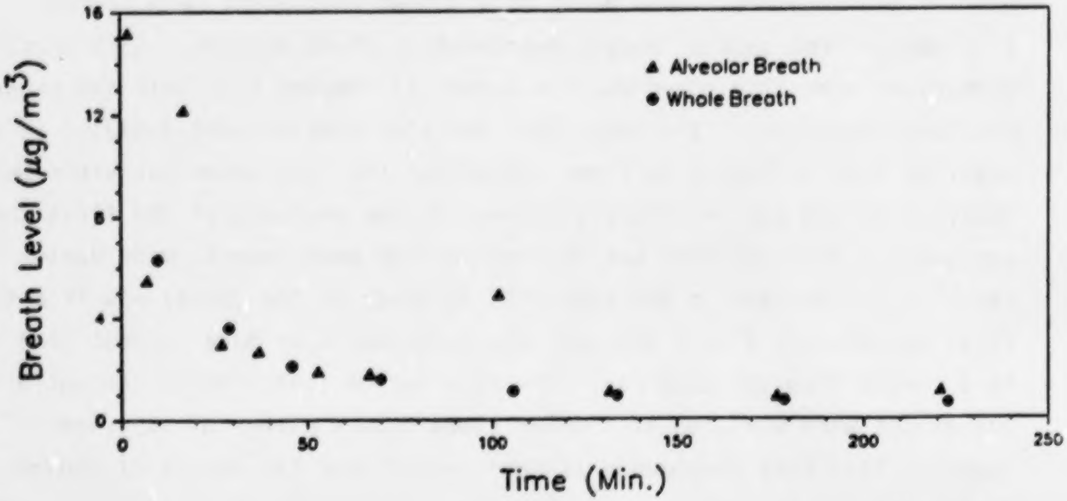

Figure 6-1B. Breath levels of m,p-xylene post exposure to furniture stripping operatations. Exposure: 240 μg/m^3; QL = 0.7 μg/m^3.

in the alveolar breath samples were observed for ethylbenzene, o-xylene, m,p-xylene and possibly toluene. Although smaller than those observed for m,p-xylene in FS1 above, these deviations might be due to contaminated canisters. We did not use the 2 L canisters in subsequent experiments where the collection of aromatic hydrocarbons was likely. The unusual curve for tetrachloroethylene (Figure E-8) might be the result of the compound elimination from multiple body compartments (see later section).

Indoor Swimming Pool (Figure E-13)--

Data from the alveolar samples provided by participant No. 2 showed decays for both chloroform and isopentane. The chloroform decay was consistent with decays measured for other organic compounds in other experiments. The isopentane decay should be interpreted with great caution because uncontrolled exposure to this compound was very likely, especially at low levels. Such levels were easily encountered while driving to the exposure site and reexposure could have occurred if there was any heavy traffic near the sample collection area.

Wood/Metal Shop (E-14 through E-16)--

This exposure experiment resulted in a very high exposure to 1,1,1-trichloroethane and the resulting decay is shown in Figure 6-2. This compound was the major component of the cutting fluid used during the last hour of the exposure. This decay also showed what might be a second elimination from another body compartment at 35-40 minutes. Such subtle elevations were also observed in a number of samples from this and other exposure situations. The individual canister samples were analyzed in the order of last collected to first collected; the last seven canisters were analyzed on the day immediately preceeding the analysis of the first three canisters. This increase was determined from measurements made during one day. If the maximum of the elevation (a break in the curve) was from the first measurement from a new day, the value would be more suspect than one in a series from the same day. The observation that similar concentration elevations were measured at similar times from a number of experiments suggests that this phenomenon is real rather than the result of random variability in the measurement technique. If random variability were the cause, the variations would also be expected to appear at random times.

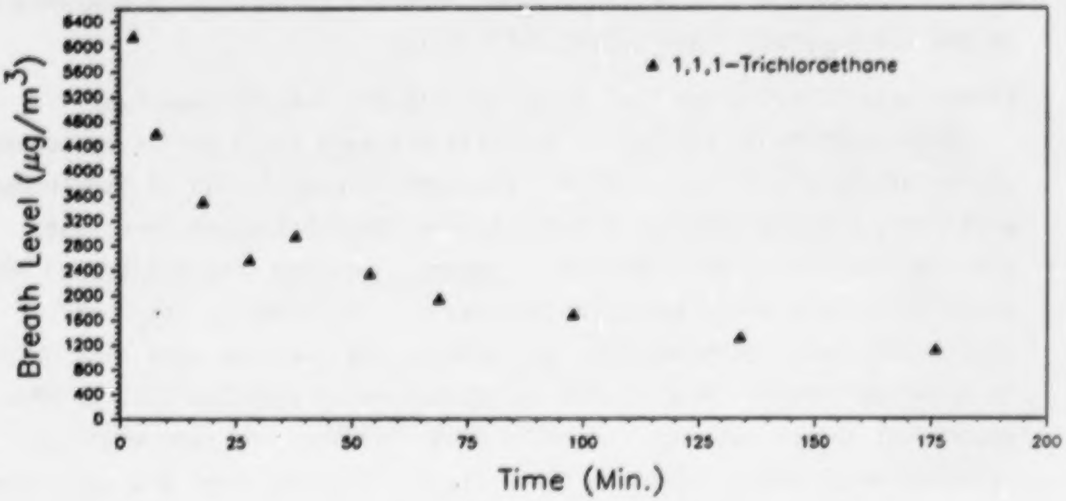

Figure 6-2. Decay of 1,1,1-trichloroethane in alveolar breath after exposure to an active wood working shop. Exposure: 16000 μg/m^3; QL = 12 μg/m^3.

This experiment also measured a decay for vinylidene chloride, that was found to be a trace component of the cutting fluid. Decays for n-pentane and toluene were also observed.

Consumer Products (Figures E-17,18)--

In this experiment, decays for limonene, α-pinene, and p-dichlorobenzene were observed. The decays for alpha-pinene and p-dichlorobenzene were quite smooth. The results for limonene were quite erratic; the reason for this is unclear, although shortterm reexposures that might not be obvious in the integrated air samples, could cause this effect. Data were not plotted beyond 17.8 hours because there was evidence of a reexposure in the air samples. (See Tables D-12, D-13)

Garage with Staining and Fuel Handling (Figures E-19 through E-32)--

This experiment resulted in the best exposure to aliphatic hydrocarbons of any of the situations studied. Moderate to high levels of isopentane, n-pentane, 2-methylpentane, 2-methylhexane, 3-methylhexane, n-octane, ethylcyclohexane, 3-methyloctane, n-nonane, n-decane, and n-undecane were measured in both whole and alveolar breath. The aromatic compounds benzene, toluene, ethylbenzene, m,p-xylene, and o-xylene were also detected at moderate levels. Most of the curves generated from the data of this experiment showed distinct secondary decay features and some even had features which might suggest a third decay. The very high exposure levels for some of these compounds could have resulted in better equilibration with deep compartments in the body, as discussed further in the section where the half life data are presented. In addition, because this was the only experiment where both the alveolar and whole breath samples were collected in 6 L canisters, thus minimizing canister volume variabilities, this data will also be the focus of the section comparing whole and alveolar breath.

Hardware Store, Second Exposure (Figures E-35 through E-42)--

Because of the variety of compounds detected in the breath after the first hardware store experiment, we chose this environment to study the effect of replicate exposure (one person two separate times) and interindividual variability (different people, same environment) on measured decays and half lives. These two topics will be discussed in a later section. The compounds detected in breath after this exposure were very similar to those found after HS1. This experiment (HS2,3) provided decay data for dichloromethane, 1,1,1-trichloroethane, toluene, ethylbenzene, m,p-xylene, n-nonane, o-xylene, and n-decane. The decay data for dichloromethane and toluene (Figures E-35 and E-36, respectively) show that participant No. 2 was emitting substantially higher levels of these two compounds even though the exposure of both participants was the same. Analytical results of the overnight air samples (Table D-17, 140HS20CF1) indicated that participant No. 2 was exposed to these two compounds at levels comparable to those measured in the hardware store during the night before the experiment. This difference in breath levels between the two participants shows that a longer exposure would result in a more complete equilibration of the body with the compounds in the exposure environments and a measurable, cumulative effect of exposure to VOCs. This has relevance for estimating different body burdens after acute vs. chronic exposure, even to low air concentrations of VOCs.

Hardware Store, Third Exposure (Figures E-43 through E-49)--

The experiment was repeated a third time with two participants different from those exposed earlier in an attempt to collect more information of interindividual variability. In this situation, dichloromethane, 1,1,1-trichloroethane, toluene, tetrachloroethylene, m,p-xylene, n-nonane, and n-decane were present in the breath at levels sufficient to provide decay information. Participant No. 3 generally had higher levels of VOCs in his breath than did participant No. 4. This might be a result of sex or body build differences between the participants as well as somewhat different exposure air concentrations for each participant (Table D-21). The data are too limited to be certain.

An interesting observation was found in the duplicate samples for participant No. 4 where the measured concentrations were often below the levels expected based on the shape of the decay curve. This was true for time points 3 and 10 minutes for dichloromethane, 1,1,1-trichloroethane, toluene, tetrachloroethylene, and n-nonane. No such trend was observed for participant No. 4. Such a situation could happen if oversampling of the exhaled breath from the spirometer were occuring. Since the total volumetric flow of 3.2 L/min (1.6 L/min into each of two 6 L canisters) was collected from the spirometer and given that this participant breathed at a faster rate (Table 4-9), which suggests a smaller alveolar volume, an oversampling situation might have occurred here. The further delopment work on this spirometer system (work assignment 50 of this contract) has indicated that a sampling flow of 1 L/min. into a 1.8 L canister should work well. Even duplicate sampling, with a total sampling flow of 2 L/min should not result in oversampling.

Comparison of Alveolar and Whole Breath

At the onset of this work, two main advantages of sampling alveolar breath with the new device over sampling whole breath with the old device were seen. First, the new spirometer design would allow for the rapid collection of samples and thus allow the elucidation of the early phase of the elimination kinetics. Second, alveolar air normally accounts for two-thirds of the tidal volume, so the concentration of VOCs in whole breath would be expected to be approximately two-thirds of the concentration in alveolar breath. All else being equal, the collection of alveolar air would be the method of choice for maximum analytical sensitivity. Although several of the exposure experiments (FS1, HS1, GS1) utilized both alveolar and whole breath collection, only GS1 collected both types of breath into canisters of the same size. Because sampling and analysis parameters were identical for both alveolar and whole breath in this experiment, data from this experiment were used for comparative purposes.

A visual comparison, with the aid of the decay plots of Figures E-19 through E-34, indicates that the consistently higher organic concentrations expected in alveolar breath were not measured. To quantify some of these differences, the concentrations in the two types of samples were directly compared at three different time points. Because the samples physically could not be collected at the same time, the concentrations for whole breath, at 12 and 185 minutes, and alveolar breath at 60 minutes were used as measured values. The corresponding concentrations in alveolar breath at 12 and 185 minutes and whole breath at 60 minutes were estimated using the equation of best fit from the bivarate curve fit analysis, discussed in the next section. For our purposes here, the estimations provided by the curve fitting routines were adequate, a conclusion supported by comparing the concentrations in Table 6-5 with the curves in Appendix E cited above. Table 6-5 presents the concentrations of each measurable compound from GS1

TABLE 6-5. PERCENT DIFFERENCE BETWEEN ALVEOLAR AND WHOLE BREATH ORGANIC COMPOUND CONCENTRATIONS AT 12, 60, AND 185 MINUTES POST-EXPOSURE[a]

	12 Min		60 Min		185 Min		(Alveolar-Whole)/ Alveolar		
	Concentrations		Concentrations		Concentrations				
Compound	Whole	Alveolar	Whole	Alveolar	Whole	Alveolar	T=12	T=60	T=185
Isopentane	180	140	71	64	38	42	-28.6	-10.9	9.5
n-Pentane	99	87	42	43	19	26	-13.8	2.3	26.9
2-Methylpentane	50	66	25	29	12	15	24.2	13.8	20.0
2-Methylhexane	44	38	11	13	8.8	7.5	-15.8	15.4	-17.3
3-Methylhexane	27	25	11	9.2	6.3	5.7	-8.0	-19.6	-10.5
Benzene	24	17	13	10	6.2	6.5	-41.2	-30.0	4.6
Toluene	40	35	22	23	8.8	15	-14.3	4.3	41.3
n-Octane	8.6	5.4	4.3	2.4	1.5	1.5	-59.3	-79.2	0.0
Ethylcyclohexane	20	24	9	11	4.9	5.5	16.7	18.2	10.9
3-Methyloctane	120	131	62	52	25	16	8.4	-19.2	-56.3
Ethylbenzene	38	36	21	26	8.5	17	-5.6	19.2	50.0
p-Xylene	23	27	11	18	4.7	7.3	14.8	38.9	35.6
n-Nonane	230	154	90	90	37	50	-49.4	0.0	26.0
o-Xylene	8.5	8.6	4.6	4.1	1.9	2.6	1.2	-12.2	26.9
n-Decane	160	143	71	83	28	55	-11.9	14.5	49.1
n-Undecane	36	61	15	23	6	11	41.0	34.8	45.5

[a] Concentration (ug/m^3) for whole breath at 12 and 185 minutes and alveolar breath at 60 minutes were as measured. The corresponding data point in whole or alveolar breath was calculated using the equation of best fit from StatPlan as in Table 6-10 or 6-12.

Both alveolar and whole breath samples were collected into 6 L canisters and analyzed in the same manner.

for both whole and alveolar breath at times 12, 60, and 185 minutes post-exposure. For clarity, the percent difference of the alveolar concentrations from the whole breath concentrations were calculated. A negative value corresponds to a situation where the alveolar breath concentration was less than the whole breath concentration.

Table 6-5 shows that only for 2-methypentane, ethylcyclohexane, _m_,_p_-xylene, and _n_-undecane were the alveolar concentrations consistently higher. In no case were the alveolar concentrations consistently lower than the whole breath concentrations. In examining the differences as function of time, it can be seen that isopentane, _n_-pentane, benzene, toluene, ethylbenzene, _n_-nonane, _o_-xylene, and _n_-decane apparently become more concentrated in the alveolar breath sample relative to the whole breath sample. The reason for this is unclear. The expected trend would be for the alveolar to be much larger than the whole breath concentrations early in the decay and assume a more constant difference later in the elimination. The reasoning behind this is that early in the elimination process the concentration is changing rapidly and the whole breath sample is integrated over several minutes thus possibly underrepresenting the concentration at the time corresponding to the start of the collection. As the changes become less rapid, the integrated values would become more accurate with regard to the actual concentration at any time during the collection of that sample and the differences between alveolar and whole breath concentrations would become constant.

Oversampling of the alveolar air could result in alveolar levels lower than the corresponding whole breath levels but this should be consistent throughout the collection of samples from a given individual. This is not the case. In addition, earlier work (task #1 of this work assignment) indicated that a sampling flow or 1.7 liters/minute should not lead to oversampling. Adsorption of the analytes to the alveolar spirometer, especially the tube, would cause the lower relative alveolar concentrations. This, too, should be consistent, especially over the small range of concentration changes measured for any given analyte in this experiment. Finally, forced exhalation, such as would occur if some resistance in the spirometer was encountered, could lead to an enrichment of the whole breath with alveolar air. That is, the percentage of deadspace air in the whole breath would decrease under these circumstances and the apparent concentration of the organic compounds would increase. Such a situation would be expected to cause the whole breath concentrations to become more similar to the alveolar concentrations. This effect would be constant over the course of the experiment.

Despite an incomplete understanding of the significance of the above phenomena noted in a single experiment, the importance of collecting breath samples in rapid succession cannot be disputed. This work has shown that the higher number of data points can more accurately describe the decay kinetics compared to collection of sequential whole breath samples. The data of Appendix C clearly indicate subtle concentration changes in the decay that are ambiguous if only whole breath data is examined. As mentioned above, these subtle changes are not likely to be artifacts.

In addition, the alveolar spirometer has the potential for being truly portable, unlike the current, whole breath spirometer, and could make the collection and analysis of breath samples very near the exposure site more feasible. The ease of use would facilitate the application of this non-invasive exposure assessment method to a much broader application than has been the case to date.

MATHEMATICAL TREATMENT OF THE DATA

This section describes the manner in which the data collected during this task was treated in order to gain information on the elimination half lives of the different organic compounds and the potential for mathematical curve fitting routines to define an equation to describe the elimination decays. The understanding of the nature of the decay for a given chemical, as measured in the breath, is a first step in the evaluation of the potential of breath analysis to predict actual exposure. What follows is a brief description of the view of the body as a multicompartment system, into which the organic compounds in air can be partitioned and eliminated at differing rates, followed by estimates of the elimination half lives of the measured compounds, assuming both a one compartment and a two compartment model, and an application of several bivariate mathematical functions to the decay data.

Compartmentalization

When a volatile organic compound is inhaled, it partitions into the blood via diffusion through the alveolar membrane. Each compound would be expected to have a distinct partition factor depending upon its volatility and solubility in the bood. Once dissolved in the blood, the compound circulates throughout the body where it can partition into other tissues, such as fat, each with a differing partition factor. The rate at which a compound can enter or exit a particular tissue depends not only on its partition factor, but also to the extent that blood flows through that tissue, i.e., the extent of perfusion. These tissues have been grouped according to the extent of perfusion and termed "compartments." Such a compartmentalized view of the body has been described by Anderson [14] and is depicted in Figure 6-3. The elimination of organic compounds from these compartments can occur at different rates. For example, a lipophilic compound such as *p*-dichlorobenzene, would be expected to be stored and released from fat tissue at a rate different from that of blood. Once the compound reenters the blood, it can partition, if it is sufficiently volatile, into the alveolar air space and be exhaled. What results during elimination is the composite clearance from these different compartments with a resulting array of elimination half-lives. Thus, the determination of the elimination kinetics and the corresponding elimination half-lives can be greatly affected by the number of compartments assumed. In this work, we considered both a one compartment and a two compartment pharmacokinetic model. The half-lives were determined using both models and the bivarate curve fitting analysis used a one compartment model.

Half-Life Estimations

In keeping with the compartmentalization models described above, the data were studied in terms of both one compartment and two compartment models consistent with the pharmacokinetic elimination of substances from the body. The measured breath concentrations and their corresponding times (post exposure) were fit to equations of the form $B = C^{-Et}$ and $B = C_1^{-E_1t} + C_2^{-E_2t}$ corresponding to a one compartment and two compartment decay, respectively, where B is the concentration in the breath at any time t, C_1 and C_2 are constants, and E is the exponential constant that determines the rate of the exponential decay. This curve fitting was accomplished using

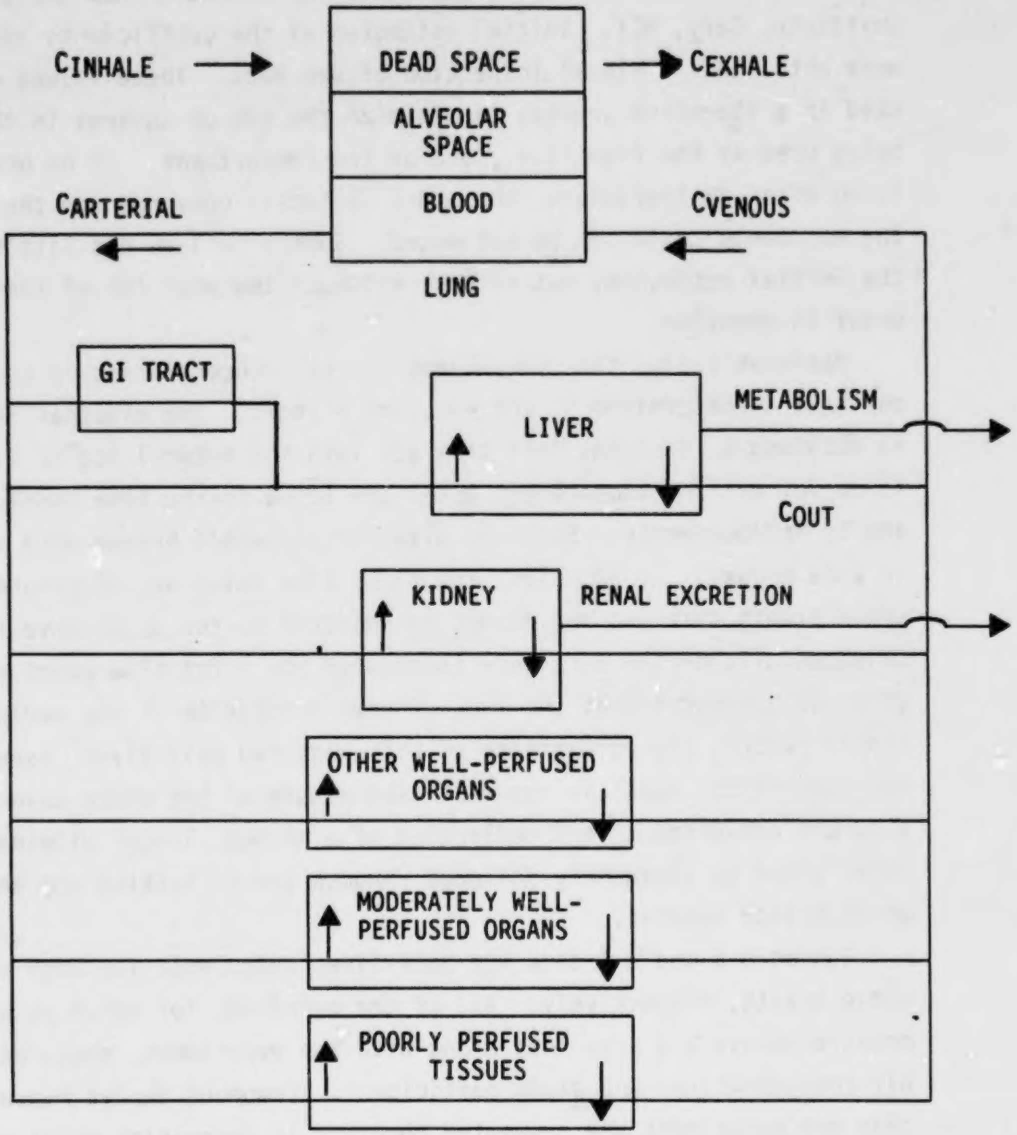
CINHALE
DEAD SPACE
CEXHALE
ALVEOLAR SPACE
CARTERIAL
BLOOD
CVENOUS
LUNG
GI TRACT
LIVER
METABOLISM
COUT
KIDNEY
RENAL EXCRETION
OTHER WELL-PERFUSED ORGANS
MODERATELY WELL-PERFUSED ORGANS
POORLY PERFUSED TISSUES

Figure 6-3. Schematic of a physiologically based model for metabolism of inhaled gases and vapors. This scheme assumes metabolism to occur only in the liver and excretion of the parent chemical to occur via the breath and to a lesser extent the kidney. Remaining tissues are grouped together on the basis of their perfusion characteristics. In a complete model each organ or set of organs has a designated volume, blood flow, and tissue:blood partition coefficient [14].

NLIN, a nonlinear curve fitting routine incorporated into SAS software (SAS Institute, Cary, NC). Initial estimates of the coefficients and exponents were obtained via visual inspection of the data. These values were then used in a iterative process to minimize the sum of squares in the model being used at the time, i.e., one or two compartment. If no minimum was found after 50 iterations, the model failed to converge and the values of the exponents could not be estimated. Such a failure has little to do with the initial estimates, but rather, reflects the poor fit of the data to the model in question.

Mathematically, the time needed for the concentration to decrease by one half is determined by the exponential term. The elimination half-life is obtained by dividing this term (E) into the natural log of 2. The half-lives for the two compartment model are found in the same manner using E_1 and E_2 independently. Both the alveolar and whole breath data were treated in this manner. In addition, the first time point was eliminated from the whole breath data and the decays resubjected to the NLIN curve fitting. If substantially better fits were found with the first time point removed, this would suggest that the lack of time resolution in the early phase simply reduces the reliability of the predicted half-lives, especially if a one compartment model is assumed. The nature of the decay associated with a second compartment, and reflective of a second, longer elimination half-life, might be adequately followed through the collection and analysis of whole breath samples.

Tables 6-6 and 6-7 show the half-lives calculated for both alveolar and whole breath, respectively. All of the compounds for which we could measure decays are presented along with the experiment, measured exposure air concentration, and study participant. Compound decays measured in more than one experiment are presented together in decreasing order of exposure concentration. They are also grouped according to compound class so that the decay behavior associated with particular chemical features, if any, could be more easily seen. Tables containing more complete information are found in Appendix F. These tables include values of R^2, which are indicative of the goodness of fit for a particular model with a value of 1 representing a perfect fit, the 95% confidence interval for the half life calculated from the confidence interval of the exponent, and an F test comparison of the one and two compartment models.

TABLE 6-6. DECAY PARAMETERS CALCULATED FROM ALVEOLAR BREATH DATA

				One Compartment Model			Two Compartment Model						
Compound	Exposure Conc. ug/m^3	Expt. Code	Participant	C_1	E_1	One Compart. $t_{1/2}$ (h)	C_1	E_1	First $t_{1/2}$ (h)	C_2	E_2	Second $t_{1/2}$ (h)	Better Fit
				Aliphatic Hydrocarbons: Straight-Chain									
n-Pentane	3400	GS1	1	126.0	0.0166	0.70	146.7	0.137	0.08	61.2	0.00494	2.34	2
n-Pentane	340	WS1	1	14.04	0.0100	1.15	8.81	0.175	0.07	10.96	0.00557	2.07	1
n-Octane	320	GS1	1	7.91	0.0172	0.67	6.87	0.0612	0.19	3.00	0.00407	2.84	2
n-Octane	39	HS2	2	2.40	0.0132	0.87	1.65	0.0678	0.17	1.22	0	IC[b]	NC[c]
n-Nonane	12000	GS1	1	175.5	0.00842	1.37	250.1	0.477	0.02	153.2	0.00688	1.73	2
n-Nonane	210	HS2	2	8.25	0.0102	1.13	8.48	0.189	0.06	5.98	0.00576	2.01	2
n-Nonane	210	HS3	1	7.09	0.0170	0.68	5.77	0.0749	0.15	3.39	0.00561	2.06	2
n-Nonane	180	HS1	2	14.46	0.132	0.08	17.05	0.626	0.02	4.79	0.0236	0.48	2
n-Nonane	130	HS4	3	19.28	0.0552	0.21	32.68	0.299	0.04	5.79	0.00756	1.53	2
n-Nonane	110	HS5	4	3.87	0.0188	0.61	CF[d]	CF	CF	CF	CF	CF	NC
n-Decane	14000	GS1	1	165.2	0.0086	1.35	85.1	0.0644	0.18	115.8	0.00495	2.33	2
n-Decane	360	HS2	2	22.49	0.0524	0.22	23.55	0.144	0.08	6.16	0.00834	1.39	2
n-Decane	360	HS3	1	16.50	0.0691	0.17	25.96	0.311	0.04	4.97	0.0110	1.06	2
n-Decane	260	HS1	2	30.64	0.129	0.08	29.87	0.161	0.07	1.91	0	IC	NC
n-Decane	210	HS4	3	31.96	0.0421	0.27	30.54	0.0605	0.19	3.83	0.00409	2.82	1
n-Decane	170	HS5	4	18.39	0.105	0.11	22.46	0.221	0.05	2.41	0	IC	NC
n-Undecane	5600	GS1	1	127.0	0.0412	0.28	139.1	0.155	0.07	43.04	0.00849	1.36	2
				Aliphatic Hydrocarbons: Branched Chain									
Isopentane	10000	GS1	1	213.3	0.0177	0.65	252.7	0.142	0.08	100.9	0.00496	2.33	2
2-Methylpentane	2000	GS1	1	83.4	0.0136	0.86	68.56	0.0556	0.21	35.78	0.00363	3.18	2
2-Methylhexane	340	GS1	1	84.8	0.0450	0.26	83.3	0.0891	0.13	16.1	0.00366	3.16	2
3-Methylhexane	410	GS1	1	45.38	0.0299	0.39	44.88	0.0899	0.13	13.25	0.00455	2.54	2
3-Methylhexane	39	FS1	1	5.67	0.0276	0.42	CF	CF	CF	CF	CF	CF	NC
2-Methyloctane	5400	GS1	1	182.2	0.0193	0.60	149.5	0.0408	0.28	53.00	0.00466	2.48	2
Ethylcyclohexane	900	GS1	1	30.38	0.0129	0.89	23.26	0.0621	0.19	15.09	0.00456	2.53	2

(continued)

TABLE 6-6 (CONT'D.)

				One Compartment Model			Two Compartment Model						
Compound	Exposure Conc. ug/m^3	Expt. Code	Participant	C_1	E_1	One Compart. $t_{1/2}$ (h)	C_1	E_1	First $t_{1/2}$ (h)	C_2	E_2	Second $t_{1/2}$ (h)	Better Fit
						Aromatic Hydrocarbons							
Benzene	430	GS1	1	18.22	0.00688	1.68	12.10	0.0855	0.14	12.69	0.00342	3.38	2
Toluene	5700	FS1	1	384.7	0.0142	0.82	295.7	0.116	0.10	231.3	0.00637	1.82	2
Toluene	1200	GS1	1	37.71	0.00627	1.84	30.81	0.223	0.05	31.35	0.00438	2.64	2
Toluene	640	HS2	2	33.39	0.00756	1.53	15.04	0.172	0.07	29.54	0.00613	1.88	1
Toluene	640	HS3	1	27.77	0.0109	1.06	19.19	0.138	0.08	20.80	0.00687	1.68	2
Toluene	510	WS1	1	21.45	0.00999	1.15	CF	CF	CF	CF	CF	CF	NC
Toluene	460	HS4	3	36.77	0.0103	1.13	67.67	0.221	0.05	21.22	0.00285	4.05	2
Toluene	320	HS1	2	25.14	0.0220	0.52	20.99	0.0441	0.27	6.31	0.00357	3.23	2
Toluene	280	HS5	4	21.26	0.00705	1.64	CF	CF	CF	CF	CF	CF	NC
Ethylbenzene	2600	GS1	1	37.67	0.00469	2.46	23.2	0.338	0.03	34.92	0.00398	2.90	2
Ethylbenzene	360	HS1	2	19.04	0.0550	0.22	17.36	0.130	0.08	4.34	0.00545	2.12	2
Ethylbenzene	150	HS2	2	2.83	0.00679	1.70	3.08	0.263	0.04	2.34	0.00464	2.49	2
Ethylbenzene	150	HS3	1	2.47	0.0113	1.02	1.14	0.150	0.08	2.04	0.00806	1.43	1
m,*p*-Xylene	1600	HS1	2	41.58	0.0127	0.92	18.81	0.410	0.03	36.09	0.0104	1.10	2
m,*p*-Xylene	1700	GS1	1	29.23	0.00721	1.60	CF	CF	CF	CF	CF	CF	NC
m,*p*-Xylene	560	HS2	2	16.42	0.0181	0.64	15.46	0.0870	0.13	7.24	0.00478	2.42	2
m,*p*-Xylene	560	HS3	1	13.90	0.0255	0.45	13.88	0.102	0.11	5.25	0.00537	2.15	2
m,*p*-Xylene	230	HS4	3	26.14	0.135	0.08	41.76	0.350	0.03	3.43	0.00533	2.16	2
m,*p*-Xylene	160	HS5	4	4.50	0.0199	0.58	5.07	0.137	0.08	2.12	0.00546	2.12	2
o-Xylene	440	HS1	2	15.19	0.0465	0.25	12.92	0.134	0.08	4.75	0.00985	1.17	1
o-Xylene	700	GS1	1	12.67	0.0172	0.67	13.66	0.103	0.11	5.32	0.00393	2.94	2
o-Xylene	190	HS2	2	2.90	0.00717	1.61	2.89	0.272	0.04	2.23	0.00116	9.95	2

(continued)

TABLE 6-6 (CONT'D.)

				One Compartment Model			Two Compartment Model						
Compound	Exposure Conc. ug/m^3	Expt. Code	Participant	C_1	E_1	One Compart. $t_{1/2}$ (h)	C_1	E_1	First $t_{1/2}$ (h)	C_2	E_2	Second $t_{1/2}$ (h)	Better Fit
					Halogenated Hydrocarbons								
Vinylidene chloride	56	WS1	1	12.27	0.00388	2.97	9.80	0.0937	0.12	8.72	0.000996	11.60	2
Dichloromethane	5000	FS1	1	299.7	0.0192	0.60	227.7	0.0859	0.13	144.3	0.00640	1.80	2
Dichloromethane	470	HS1	2	64.62	0.0283	0.40	45.02	0.121	0.10	31.16	0.0108	1.07	2
Dichloromethane	460	HS3	1	26.17	0.0108	1.07	23.45	0.0147	0.78	3.50	0	IC	NC
Dichloromethane	320	HS4	3	45.20	0.0177	0.65	27.41	0.142	0.08	31.94	0.0101	1.14	2
Dichloromethane	220	HS5	4	23.11	0.006	1.86	3.03	0.0695	0.17	21.64	0.00559	2.07	1
Chloroform	600	SP1	2	69.44	0.0161	0.72	49.82	0.125	0.08	42.70	0.00731	1.58	2
1,1,1-Trichloroethane	16000	WS1	1	5150.1	0.0131	0.88	4316.7	0.123	0.10	3223.4	0.00608	1.90	2
1,1,1-Trichloroethane	340	HS1	2	73.15	0.00940	1.22	46.76	0.0903	0.13	47.09	0.00445	2.60	2
1,1,1-Trichloroethane	200	HS2	2	107.7	0.00269	4.33	12.33	0	0.00	95.43	0.00303	3.81	1
1,1,1-Trichloroethane	200	HS3	1	42.93	0.0117	0.99	36.14	0.0697	0.17	22.18	0.00363	3.18	2
1,1,1-Trichloroethane	200	HS5	4	26.52	0.0034	3.39	10.82	0.0697	0.17	22.01	0.00190	6.08	1
1,1,1-Trichloroethane	140	FS1	1	46.94	0.0115	1.00	30.56	0.145	0.08	33.65	0.00644	1.80	2
Trichloroethylene	77	FS1	1	6.41	0.0176	0.65	4.70	0.058	0.20	2.53	0	IC	NC
Tetrachloroethylene	280	HS1	2	45.81	0.00477	2.42	14.64	0.0601	0.18	37.54	0.00311	3.70	2
Tetrachloroethylene	190	HS4	3	57.33	0.0137	0.85	40.79	0.105	0.11	37.08	0.00693	1.67	2
Tetrachloroethylene	150	HS5	4	22.47	0.00559	2.06	CF	CF	CF	CF	CF	CF	NC

[a] Model showing better fit based on the F-test at the 95% confidence interval. 1 = one compartment, 2 = two compartment.

[b] IC = data reflected insufficient change in concentration to calculate a second half-life over this time interval.

[c] NC = not calculated.

[d] CF = convergence failure; residuals failed to converge in 50 steps during iterative computation and reflects the poor fit of the data to the model in question.

TABLE 6-7. DECAY PARAMETERS CALCULATED FORM WHOLE BREATH DATA

				One Compartment Model			Two Compartment Model						
Compound	Exposure Conc. ug/m^3	Expt. Code	Participant	C_1	E_1	One Compart. $t_{1/2}$ (h)	C_1	E_1	First $t_{1/2}$ (h)	C_2	E_2	Second $t_{1/2}$ (h)	Better Fit
				Aliphatic Hydrocarbons: Straight-Chain									
n-Pentane	3400	GS1	1	104.7	0.0132	0.88	95.77	0.0443	0.26	46.13	0.00499	2.32	2
n-Octane	320	GS1	1	9.25	0.0122	0.95	1.23	0	0.00	9.03	0.0190	0.61	1
n-Nonane	12000	GS1	1	264.4	0.0157	0.74	257.1	0.0278	0.42	49.8	0.00208	5.55	2
n-Decane	14000	GS1	1	175.58	0.0131	0.88	110.9	27.2	0.00	175.6	0.0131	0.88	1
n-Undecane	5600	GS1	1	38.24	0.0135	0.86	32.41	0.0594	0.19	21.88	0.00718	1.61	2
				Aliphatic Hydrocarbons: Branched-Chain									
Isopentane	10000	GS1	1	185.5	0.0130	0.89	190.3	0.0472	0.24	76.7	0.00406	2.85	2
2-Methylpentane	2000	GS1	1	51.3	0.0113	1.02	43.01	0.0448	0.26	26.82	0.00514	2.25	2
2-Methylhexane	340	GS1	1	28.4	0.0133	0.87	28.51	0.0398	0.29	9.996	0.00333	3.47	2
3-Methylhexane	400	GS1	1	28.53	0.0131	0.88	27.81	0.0370	0.31	9.77	0.00324	3.57	2
2-Methyloctane	5400	GS1	1	134.4	0.0121	0.96	121.2	0.0204	0.57	28.40	0.00222	5.20	1
				Cyclic Hydrocarbons									
Ethylcyclohexane	900	GS1	1	21.17	0.0116	0.99	19.51	0.0292	0.40	6.55	0.00174	6.64	2
α-Pinene	97	CP1	2	26.26	0.877	0.79	4.10	5.33	0.13	3.74	0.433	1.60	2
Limonene	160	CP1	2	5.35	0.2857	2.43	3.19	2.87	0.24	3.63	0.1007	6.88	1

(continued)

TABLE 6-7 (CONT'D.)

				One Compartment Model			Two Compartment Model						
Compound	Exposure Conc. ug/m^3	Expt. Code	Participant	C_1	E_1	One Compart. $t_{1/2}$ (h)	C_1	E_1	First $t_{1/2}$ (h)	C_2	E_2	Second $t_{1/2}$ (h)	Better Fit
Aromatic Hydrocarbons													
Benzene	430	GS1	1	24.44	0.00887	1.30	19.16	0.0250	0.46	10.26	0.00280	4.12	2
Toluene	5700	FS1	1	293.5	0.0112	1.03	216.8	0.0369	0.32	145.1	0.00507	2.28	2
Toluene	1200	GS1	1	41.90	0.00935	1.24	20.81	0.0370	0.31	28.93	0.00620	1.86	2
Toluene	320	HS1	2	13.70	0.0113	1.03	CF[d]	CF	CF	CF	CF	CF	NC[c]
Ethylbenzene	2600	GS1	1	40.10	0.00922	1.25	24.64	0.024	0.48	20.84	0.00471	2.45	2
Ethylbenzene	360	HS1	2	6.24	0.0121	0.95	4.72	0.0470	0.25	3.20	0.00532	2.17	2
m,p-Xylene	1600	HS1	2	21.21	0.0110	1.05	12.09	0.0640	0.18	14.87	0.00719	1.60	2
m,p-Xylene	1700	GS1	1	24.56	0.0109	1.06	21.47	0.0223	0.52	6.90	0.00233	4.98	2
m,p-Xylene	240	FS1	1	7.28	0.0211	0.55	7.41	0.0446	0.25	1.65	0.00460	2.52	2
o-Xylene	440	HS1	2	4.91	0.0124	0.93	4.63	0.1322	0.08	3.50	0.00780	1.48	2
o-Xylene	700	GS1	1	8.83	0.00958	1.21	7.59	0.0216	0.53	2.74	0.00192	6.02	2
Halogenated Hydrocarbons													
Dichloromethane	5000	FS1	1	212.6	0.0121	0.95	203.8	0.0284	0.40	54.66	0.00145	7.98	2
Dichloromethane	470	HS1	2	48.95	0.0207	0.55	47.73	0.0337	0.33	7.11	0.00213	5.40	2
1,1,1-Trichloroethane	340	HS1	2	49.55	0.00861	1.33	39.71	0.0137	1.38	10.58	0	IC[b]	NC
1,1,1-Trichloroethane	140	FS1	1	31.34	0.0105	1.10	28.60	0.0222	0.52	7.38	0	IC	NC
Tetrachloroethylene	280	HS1	2	35.96	0.00541	2.13	27.77	0.00685	1.68	6.93	0	IC	NC
p-Dichlorobenzene	9400	CP1	2	309.9	0.442	1.57	260.2	1.30	0.53	103.3	0.0326	21.00	2

[a] Model showing better fit based on the F-test at the 95% confidence interval. 1 = one compartment, 2 = two compartment.

[b] IC = data reflected insufficient change in concentration to calculate a second half-life over this time interval.

[c] NC = not calculated.

[d] CF = convergence failure; residuals failed to converge in 50 steps during iterative computation and reflects the poor fit of the data to the model in question.

Almost without fail, the two compartment model was better able to accurately describe the measured decays. This is illustrated for the decay of dichloromethane (experiment FS1) in alveolar breath and whole breath for both the one compartment model, Figure 6-4, and the two compartment model, Figure 6-5. In both cases, the actual data are shown as points on a ln-linear scale along with the similarly transformed theoretical equation that appears as a solid curve. If the data were a perfect match to the theoretical in a one compartment model (Fig. 6-4), all of the points would fall on a straight line. This is clearly not the case for the dichloromethane data in either alveolar or whole breath. A perfect fit in the two compartment case would result in the data falling exactly onto an exponential curve. Figure 6-5 shows that the two compartment description of the decay is a far better fit than was the one compartment case. The differing curve shapes in the two compartment case for alveolar and whole breath suggest that an inadequate definition of the first phase decay i.e., whole breath, alters the predicted half life.

The half-lives calculated for whole breath when the first data point was removed from the set are shown in Table 6-8 for data from the garage experiment. For the one compartment model, the removal of the first time point resulted in the estimated half-lives becoming longer suggesting that a failure to measure data from the early phase of the elimination can skew the results. With the two compartment model, the reduction of the data set size caused a significant number of convergence failures. As described above, this implies that the data no longer fit a two compartment model very well. Because the F test results with full data sets (Appendix F) show that the two compartment model is generally superior to the one compartment model, we can conclude that data points collected early in the elimination decay are crucial to the accurate representation of the decay.

Observations Regarding the Dependence of Half Life on Exposure Level and Study Participant--

One question we asked at the beginning of this study was whether or not the measured half-life was dependent upon the level of exposure. This question is particularly relevent if elimination half-lives are to be used in a model to predict exposure based on post exposure breath measurements. To answer this question, refer to the measured half-lives for toluene and

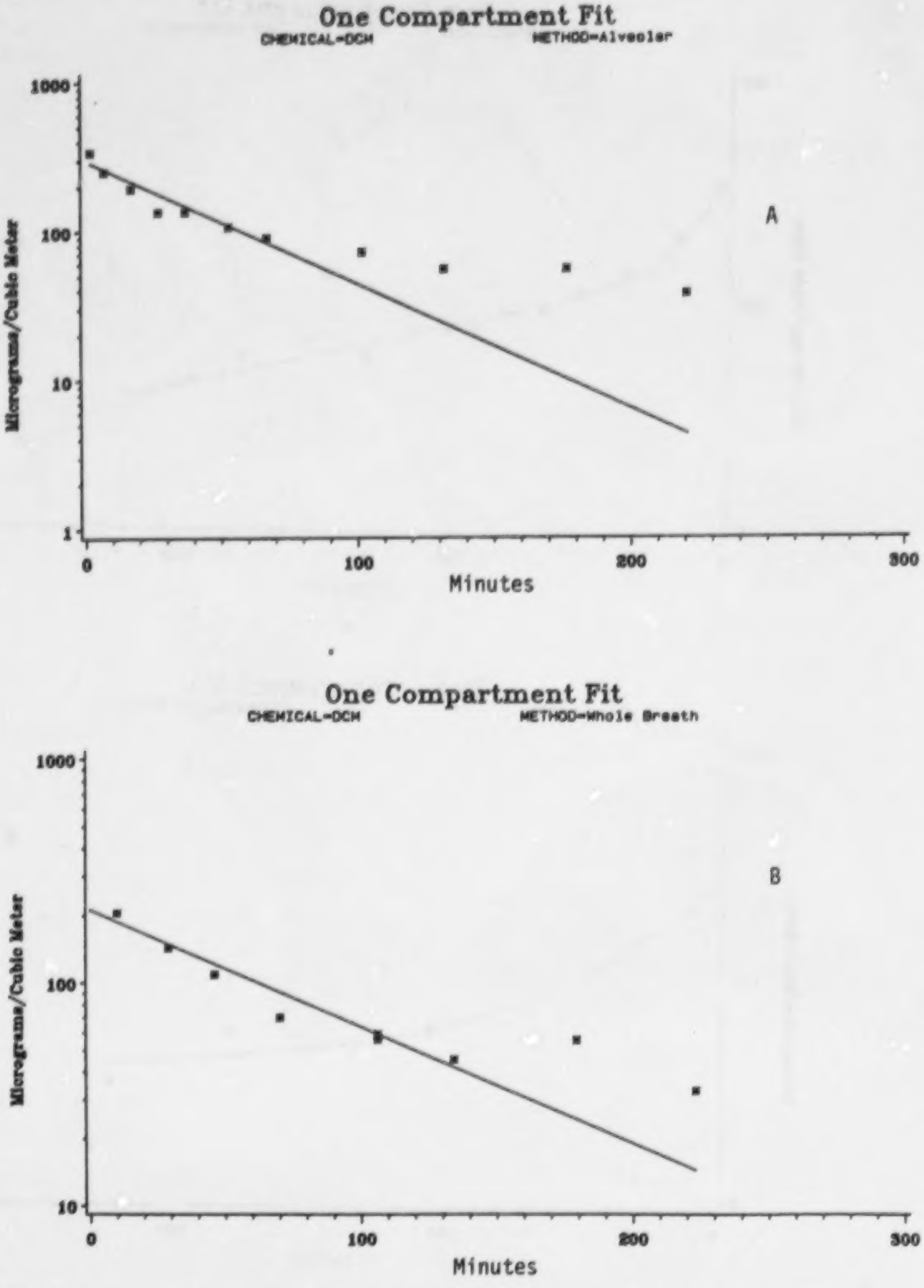

Figure 6-4. Ln-linear display of decay data measured for dichloromethane in alveolar (A) and whole (B) breath. The solid line indicates a curve defined by data showing an ideal fit to a one compartment model.

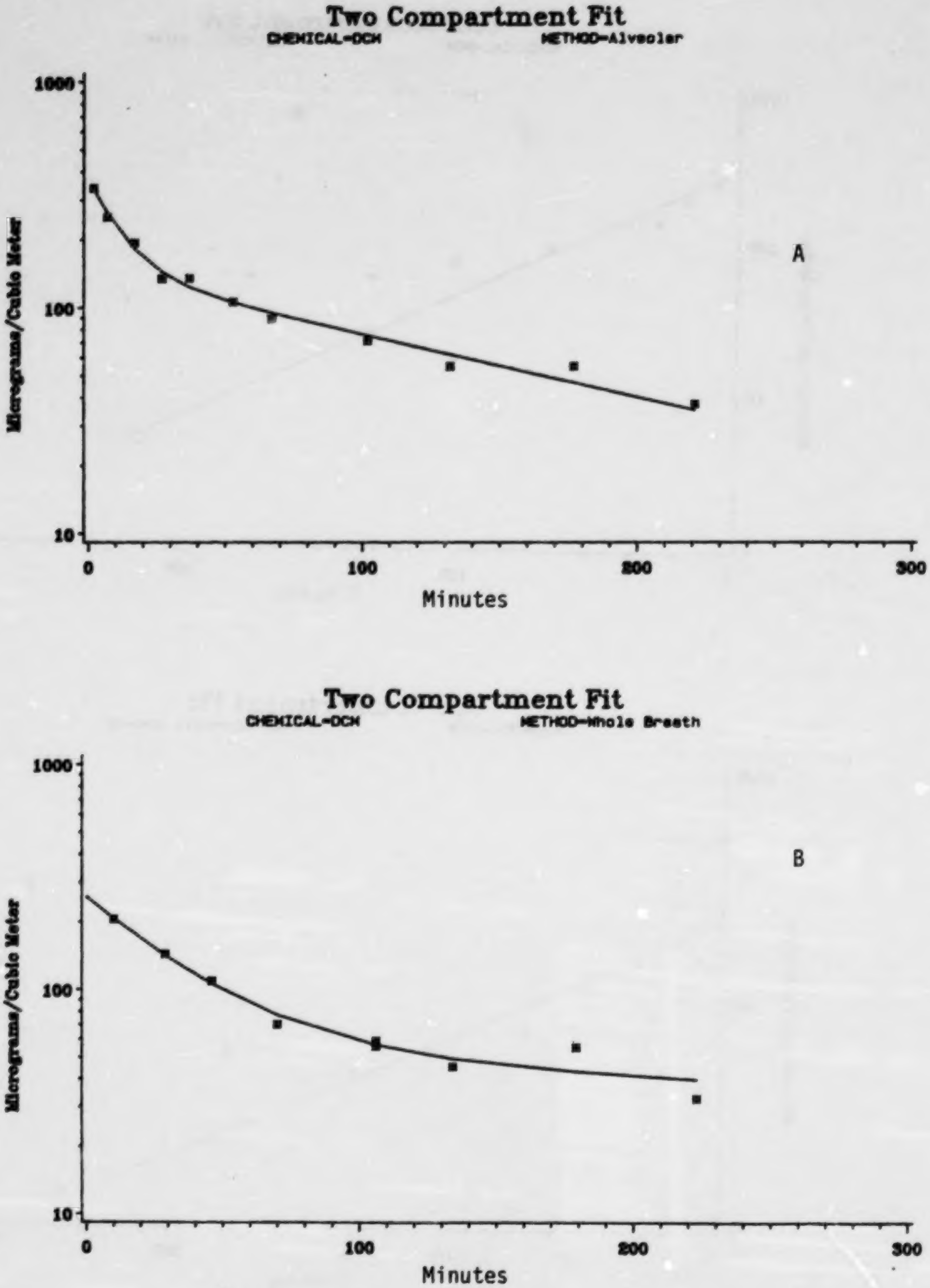

Figure 6-5. Ln-linear display of decay data measured for dichloromethane in alveolar (A) and whole (B) breath. The solid curve indicates a curve defined by data showing an ideal fit to a two compartment model.

TABLE 6-8. COMPARISON OF CALCULATED HALF-LIVES FOR WHOLE BREATH DATA WITH AND WITHOUT FIRST TIME POINT (GARAGE EXPERIMENT)

		One Compartment		Two Compartment			
Compound	Exposure Conc.[a] ug/m^3	$t_{1/2}$ With	$t_{1/2}$ Without	First $t_{1/2}$ With	Second $t_{1/2}$ With	First $t_{1/2}$ Without	Second $t_{1/2}$ Without
Isopentane	10,000	0.89	1.47	0.24	CF[b]	2.85	CF
Pentane	2,000	0.88	1.29	0.26	CF	2.32	CF
2-Methylpentane	1,200	1.02	1.44	0.26	CF	2.25	CF
2-Methylhexane	550	0.87	1.37	0.29	0.01	3.47	1.37
3-Methylhexane	340	0.88	1.36	0.31	0.13	3.57	2.31
Benzene	250	1.30	1.60	0.46	0.29	4.12	2.79
Toluene	740	1.24	1.43	0.31	CF	1.86	CF
Ethylcyclohexane	590	0.99	1.32	0.40	0.12	6.64	2.17
2-Methyloctane	3,800	0.96	1.05	0.57	0.12	5.20	1.53
Ethylbenzene	1,500	1.25	1.42	0.48	CF	2.45	CF
p-Xylene	1,000	1.06	1.27	0.52	0.34	4.98	2.64
o-Xylene	420	1.21	1.45	0.53	CF	6.02	NC
n-Octane	320	0.95	1.18	0.61	2.9×10^{-4}	CF	1.18
n-Nonane	7,100	0.74	0.94	0.42	6.7×10^{-5}	5.55	0.94
n-Decane	8,200	0.88	1.11	4×10^{-4}	0.17	0.88	1.81
n-Undecane	3,200	0.86	1.23	0.19	0.67	1.61	10.4

[a] Exposure concentrations are approximate.

[b] CF = convegence; residuals failed to converge in 50 steps during interactive computation.

dichloromethane of Table 6-6. No consistent correlation of half-life with exposure level is observed. The data, however, are quite limited which makes a definitive statement impossible. A lack of dependence on the level of exposure would support the use of half-life in a predictive process.

Two other important questions are (1) what is the observed variability in the measured half lives for a particular compound within one individual? and (2) what is the observed variability between individuals for exposure to the same compound? For those compounds which were measured in several experiments, the results in Table 6-6 suggest that in some cases the intra- and interindividual variability is small and in other cases the variability is larger. Because of the limited number of observations, no firm conclusions can be drawn. The fact that in many cases intra- and interindividual variabilities were small suggests that further evaluations are required. Experiments where several people are exposed several times at several different levels could be designed to address this question.

Practical Results of This Work

Without question, one of the main results of this work is that significant exposure to a variety of volatile organic compounds can occur in a variety of everyday situations. Beyond this, we have demonstrated that exposures are, in many cases, high enough to characterize elimination decays of VOCs in breath. This is significant in that elimination half-lives can be mesured without using exposure chambers which should allow more widespread study of elimination kinetics.

The alveolar breath sampling device developed and used during this work has also proven to be very useful. The ability to collect many samples in rapid succession beginning just after exposure cessation greatly improves the quality of the data needed to accurately represent the decay profile. In addition, this device could be further developed so that it is rendered more portable and even simpler to use than was the case in this work. Such development has the capability of expanding the application of breath measurements and its potential use as a noninvasive exposure assessment tool.

Bivariate Curve Fitting Results

A knowledge of the kinetics of the elimination of a VOC from the body through the breath can provide a foundation for the mathematical description of this process and its eventual use in predicting recent exposure. Towards that end, we studied how well each data set fit each of six bivariate equations incorporated into the software package "StatPlan III" published by The Futures Group of Glastonbury, CT. In each case, the time post-exposure at which the sample was collected was the independent variable and the measured breath concentration of the particular VOC was the dependent variable. The equations used are shown in Table 6-9. For illustrative purposes, the fit of the alveolar n-pentane decay data from the GS1 experiment is shown for each equation type in Figures 6-6 through 6-12. In each case the experimental data are represented as distinct points along with the best possible curve permitted by an equation of that type as a solid line. The value of R^2, a measure of the goodness of fit, is included for reference. For the case of this pentane decay, the power function best described the observed curve.

The treatment of the decay data in this manner was done solely to study how other mathematical descriptions might apply. Unlike the exponential equations described above, these mathematical functions, to the best of our knowledge, do not have a physical basis. This fact would not diminish the ability of the function to describe the decay but would alter the manner in which it was interpreted with regard to the physiological process.

The curves of best fit for the decays measured in alveolar air are listed in Table 6-10. It should be stressed here that these equations all assume a one compartment scenario. In all cases, the two compartment, exponential equations discussed above provided a higher R^2 value and, hence, a better fit than these one compartment description. Each target compound is listed along with the experiment in which it was measured and the participant providing the data. The experiments are listed in decresing order of exposure level to make any trends related to exposure level more evident. The power, inverse concentration, and natural log functions appeared most frequently as the best fit. The equation that provides the best fit as measured by the R^2 value can be deceptive insofar as the predictive value of the curve is concerned. For example, Table 6-11 shows the residual (actual value - predicted value) as a percentage difference from the actual value for 1,1,1-trichloroethane from experiment WS1 (alveolar breath) for two curves. The inverse concentration function indicated an R^2 of 0.974 and the Ln function indicated an R^2 of 0.973; each

TABLE 6-9. MATHEMATICAL FUNCTIONS USED IN THE BIVARIATE CURVE FIT ANALYSES

Curve Type	Mathematical Description
Linear	$C = mt + b$
Exponential	$\ln C = mt + b$
Power	$\ln C = m\ln t + b$
Logarithmic	$C = m\ln t + b$
Inverse C	$1/C = mt + b$
Inverse t and C	$1/C = m/t + b$
Inverse t	$C = m/t + b$

Where:
C = value of dependent variable (concentration)
t = value of independent variable (time)
m = slope
b = intercept

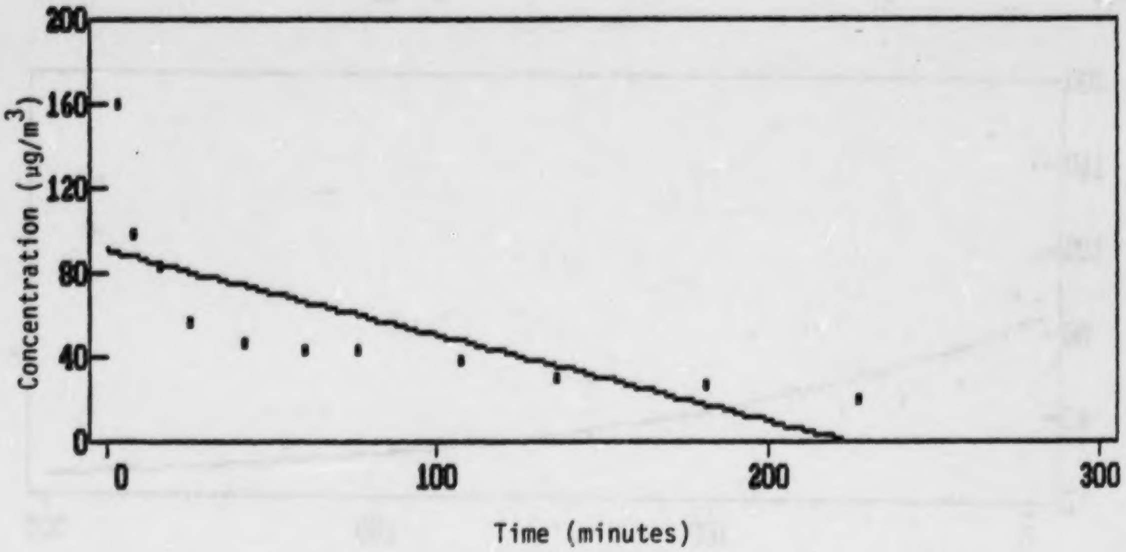

Figure 6-6. Concentration of n-pentane in alveolar breath as a function of time post exposure. Decay data fit to the linear function. R2 = 0.538.

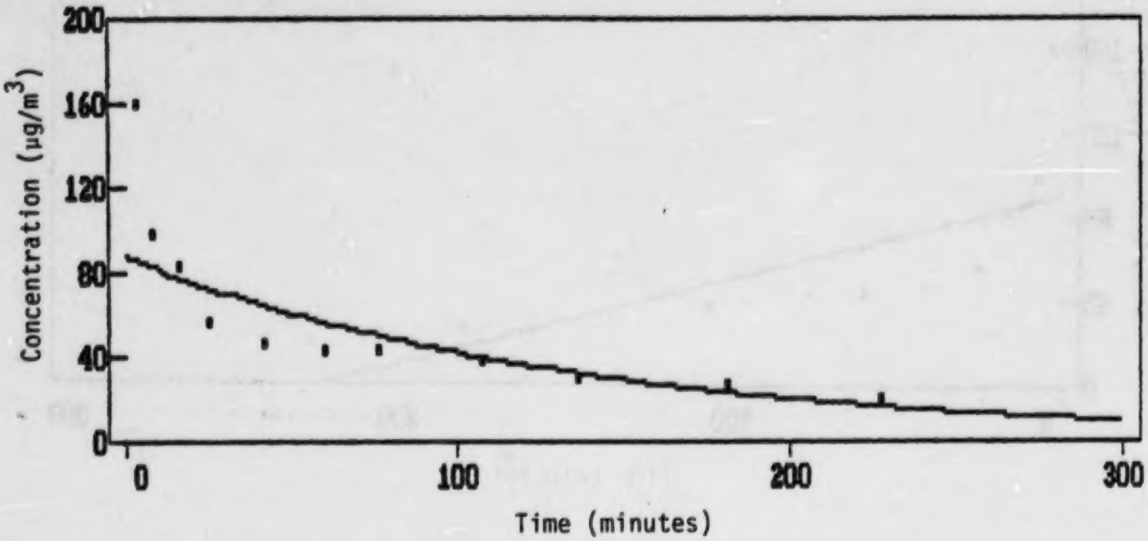

Figure 6-7. Concentration of n-pentane in alveolar breath as a function of time post exposure. Decay data fit to the exponential function. $R^2 = 0.803$.

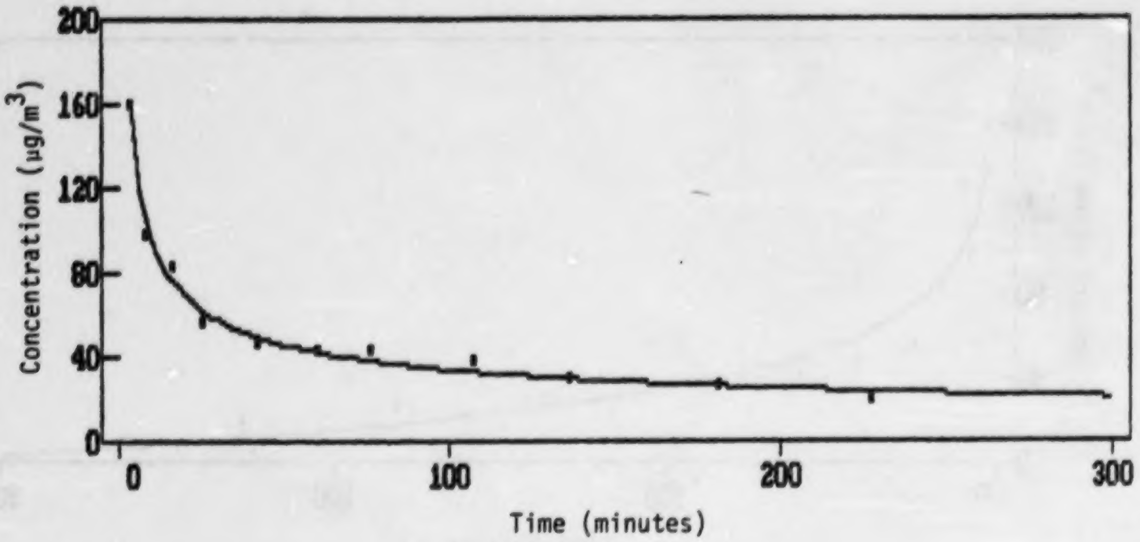

Figure 6-8. Concentration of n-pentane in alveolar breath as a function of time post exposure. Decay data fit for the power function. $R^2 = 0.977$.

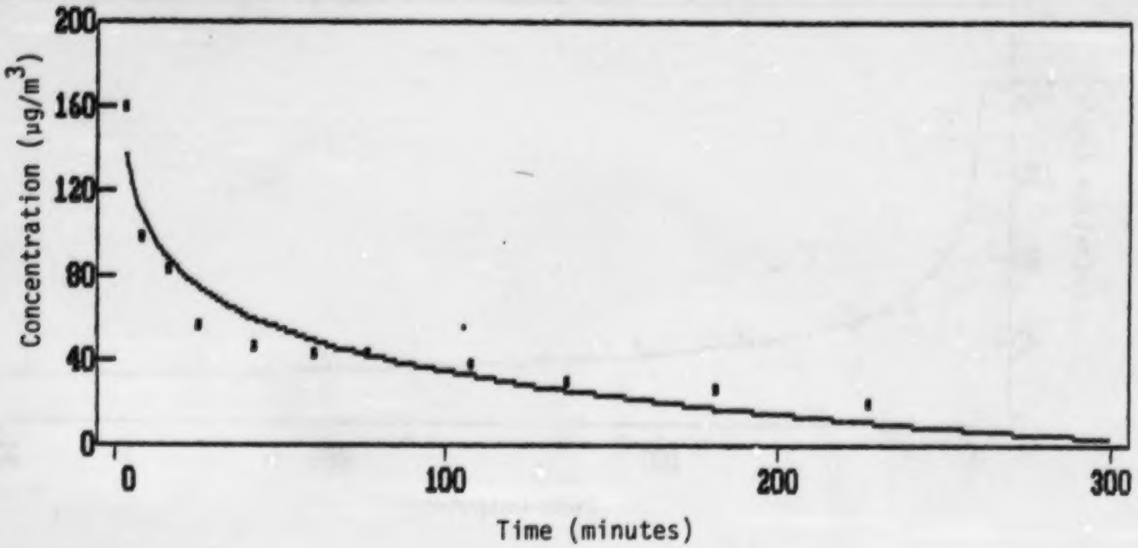

Figure 6-9. Concentration of n-pentane in alveolar breath as a function of time post exposure. Decay data fit to the natural log function. $R^2 = 0.919$.

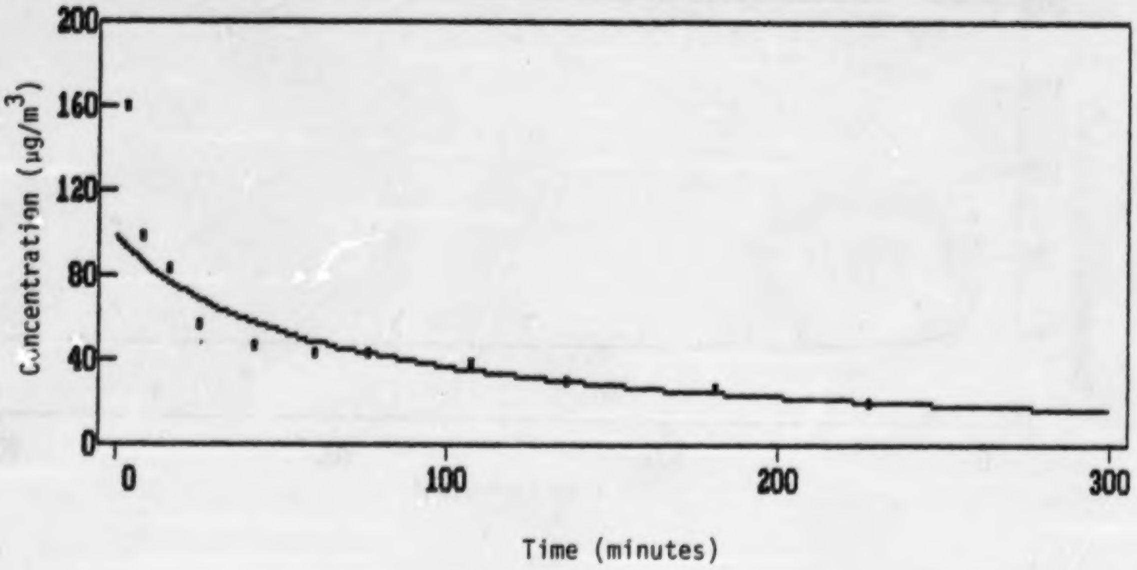

Figure 6-10. Concentration of n-pentane in alveolar breath as a function of time post exposure. Decay data fit to the inverse concentration function. $R^2 = 0.959$.

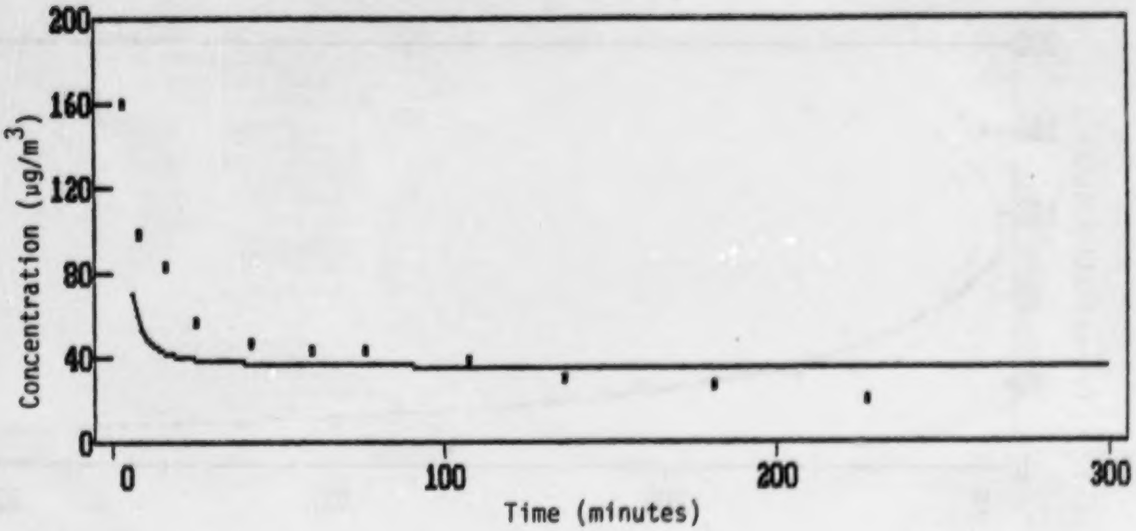

Figure 6-11. Concentration of n-pentane in alveolar breath as a function of time post exposure. Decay data fit to the inverse concentration and time function. $R^2 = 0.430$.

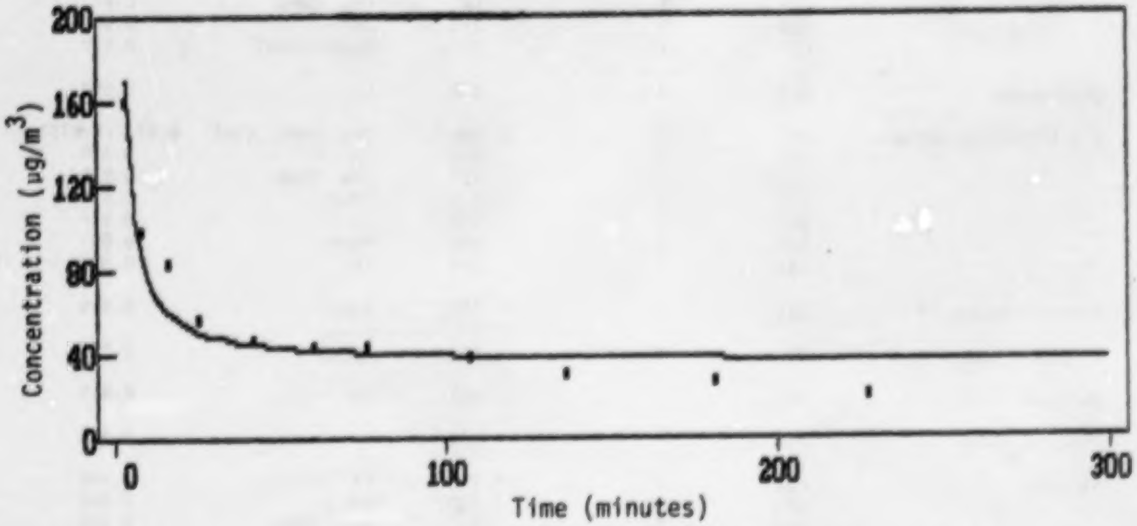

Figure 6-12. Concentration of n-pentane in alveolar breath as a function of time post exposure. Decay data fit to the inverse time function. $R^2 = 0.920$.

TABLE 6-10. RESULTS OF STATPLAN BIVARIATE CURVE-FITTING SURVEY FOR ALVEOLAR BREATH SAMPLES

Compound	Experiment	Participant	Exposure Level[a] (ug/m^3)	Best Fit	R^2
Isopentane	GS1	1	10,000	Power	0.971
Pentane	GS1	1	3,400	Power	0.977
	WS1	1	440	Inv. conc.	0.718
Vinylidene Chloride	WS1	1	56	Ln	0.863
2-Methylpentane	GS1	1	2,000	Ln	0.964
Dichloromethane	FS1	1	>5,000	Ln	0.983
	HS1	2	480	Inv. conc.	0.995
	HS2[b]	2	450	Ln	0.956
	HS3	1	450	Inv. conc.	0.977
	HS4	3	270	Ln	0.995
	HS5	4	270	Exponential	0.939
Chloroform	SP1	2	600	Ln	0.987
1,1,1-Trichloroethane	WS1	1	18,000	Inv. conc. (ln)	0.974 (0.973)
	HS1	2	330	Ln	0.996
	HS4[b]	3	210	Inv. time	0.955
	HS5	4	210	Power	0.817
	HS2	2	200	Ln	0.916
	HS3	1	200	Power	0.987
	FS1	1	120	Ln	0.993
2-Methylhexane	GS1	1	340	Power	0.926
3-Methylyhexane	GS1	1	406	Power	0.982
Benzene	GS1	1	427	Ln	0.949
Trichloroethylene	FS1	1	13	Ln	0.966
Toluene	FS1	1	5,700	Ln	0.982
	GS1	1	1,200	Ln	0.969
	HS2	2	640	Inv. conc.	0.965
	HS3	1	640	Inv. conc.	0.990
	WS1	1	510	Inv. conc.	0.954
	HS4	3	370	Inv. time	0.979
	HS5	4	370	Ln	0.880
	HS1	2	320	Inv. conc.	0.967
n-Octane	GS1	1	320	Power	0.965
Tetrachloroethylene	HS1	2	260	Inv. conc.	0.952
	HS4	3	170	Ln	0.983
	HS5	4	170	Inv. time	0.840
Ethylcyclohexane	GS1	1	900	Ln	0.981
3-Methyloctane	GS1	1	5,400	Ln	0.971
Ethylbenzene	GS1	1	2,610	Inv. conc.	0.961
	HS1	2	470	Power	0.934
	HS2	2	150	Inv. conc.	0.923
	HS3	1	150	Inv. conc.	0.963
m,*p*-Xylene	GS1	2	1,600	Exponential	0.961
	HS1	1	1,700	Exponential	0.944
	HS2	2	570	Inv. conc.	0.933
	HS3	1	570	Inv. conc.	0.967
	HS4	3	190	Inv. time	0.985
	HS5	4	190	Ln	0.875

(continued)

TABLE 6-10 (cont'd.)

Compound	Experiment	Participant	Exposure Level ($\mu g/m^3$)	Best Fit	R^2
n-Nonane	GS1	1	12,020	Inv. conc.	0.983
	HS2	2	200	Power	0.960
	HS3	1	200	Power	0.956
	HS1	2	160	Power	0.989
	HS4	3	120	Inv. time	0.983
	HS5	4	120	Ln	0.900
o-Xylene	GS1	2	440	Ln	0.911
	HS1	1	701	Power	0.973
	HS2	2	200	Inv. time	0.974
n-Decane	GS1	1	13,800	Ln	0.955
	HS2	2	330	Inv. conc.	0.929
	HS3	1	330	Inv. time	0.989
	HS1	2	280	Inv. conc.	0.980
	HS4	3	190	Power	0.921
	HS5	4	190	Inv. time	0.989
n-Undecane	GS1	1	5,600	Power	0.991

[a] Exposure levels for garage experiment (GS1) as approximate.

[b] Significant exposure occurred during the night before the exposure experiment.

TABLE 6-11. COMPARISON OF PREDICTIVE ABILITIES OF TWO FUNCTIONS FOR THE DECAY OF 1,1,1-TRICHLOROETHANE IN ALVEOLAR BREATH (EXPERIMENT WS1)

	% Difference from Measured	
Time Post-Exposure (min)	Inverse Concentration (R^2 = 0.974)	Ln (R^2 = 0.973)
3	30	6
8	13	-0.6
18	2	-5
28	-20	-23
38	6	5
54	-1	-1
69	-8	-8
98	-2	0.3
134	-6	-0.008
176	-2	11
218	6	28

provides more accurate predictions in different portions of the curve. The inverse concentration function clearly performs better at longer times while the Ln function handles the early time points better. Some of the time points are very accurately predicted. The elevation in breath concentration measured at 28 minutes, presumably related to a second physiological compartment, is not effectively predicted by either function. From this we can conclude that the predictive power of each function cannot be gleaned from R^2 alone and that more complex mathematical functions will be required to very accurately predict multicompartment systems.

The analogous results for the whole breath data are shown in Table 6-12. As for the half-life determinations, the whole breath data were first subjected to the curve fitting analysis with all of the data points included and then with the first time point eliminated from the data set. When all of the data points were included in the analyses, the most frequently selected curves were power, Ln, and inverse concentration. When the first point was eliminated, inverse concentration and inverse time became the dominant functions. This supports the idea that the early time points are very important in accurately defining the elimination of an organic compound from the body. Table 6-13 presents the % difference of the predicted value from the actual value for the benzene decay of experiment GS1 for whole breath (all data points and without the first point) and alveolar breath. The comparison of actual vs. predicted concentration values for whole breath indicated that the best-fit equation could predict the actual values quite well. Through the elimination of the first data point, the values were predicted with only a 4% deviation compared to the 8% for the case when all points were included but such an analysis clearly fails to provide information on the early-phase elimination. The alveolar data indicate that as the number of data points increases and the resulting curve contains more subtleties, the mathematical functions required to accurately define the curve become more complex.

TABLE 6-12. RESULTS OF STATPLAN BIVARIATE CURVE-FITTING SURVEY FOR WHOLE BREATH SAMPLES

Compound	Experiment	Participant	Exposure Level[a] (ug/m^3)	Best Fit (All)	R^2	Best Fit (Less 1st pt.)	R^2
Isopentane	GS1	1	10,100	Power	0.983	Power	0.972
n-Pentane	GS1	1	3,440	Inv. conc.	0.985	Inv. conc.	0.981
2-Methylpentane	GS1	1	1,990	Ln	0.966	Inv. time	0.952
Dichloromethane	FS1	1	>5000	Ln	0.957	Inv. time	0.967
	HS1	2	480	Power	0.963	Inv. time	0.987
1,1,1-Trichloroethane	HS1	2	330	Ln	0.972	Inv. time	0.947
	FS1	1	120	Ln	0.982	Power	0.967
2-Methylhexane	GS1	1	342	Power	0.965	Inv. time	0.965
3-Methylhexane	GS1	1	406	Power	0.970	Inv. time	0.982
Benzene	GS1	1	427	Inv. conc.	0.991	Power	0.995
Toluene	FS1	1	5700	Inv. conc.	0.997	Inv. conc.	0.996
	GS1	1	1,240	Ln	0.988	Inv. conc.	0.985
	HS1	2	320	Ln	0.967	Inv. conc.	0.932
n-Octane	GS1	1	319	Ln	0.966	Inv. conc.	0.950
Tetrachloroethylene	HS1	2	260	Ln	0.965	Inv. time	0.915
Ethylcyclohexane	GS1	1	590	Ln	0.981	Inv. time	0.989
3-Methyloctane	GS1	1	3,800	Ln	0.973	Inv. time	0.985
Ethylbenzene	GS1	1	2,610	Ln	0.990	Inv. conc.	0.989
	HS1	2	470	Ln	0.981	Power	0.966
m,*p*-Xylene	HS1	2	1,600	Ln	0.988	Ln	0.969
n-Nonane	GS1	1	12,800	Inv. conc.	0.987	Inv. time	0.992
o-Xylene	HS1	2	440	Ln	0.989	Exponential	0.993
n-Decane	GS1	1	13,800	Inv. conc.	0.998	Inv. conc.	0.998
n-Undecane	GS1	1	5,600	Inv. conc.	0.996	Inv. conc.	0.994
α-Pinene	CP1	2	95	Ln	0.997	Ln	0.998
p-Dichlorobenzene	CP1	2	10,000	Power	0.967	Power	0.988
Limonene	CP1	2	160	Power	0.881	Inv. time	0.837

[a] Exposure levels for garage experiment (GS1) are approximate.

TABLE 6-13. EFFECT OF DATA SET COMPLETENESS ON PREDICTIVE ABILITIES OF FITTED BIVARIATE CURVES FOR BENZENE (EXPERIMENT GS1)

	% Difference from Measured		
Time Post-Exposure (min)	Whole (All Points)[a]	Whole (Less First Point)[b]	Alveolar (All Points)[c]
3	-[d]	-	6
8	-	-	-12
12	8	-[e]	-
16	-	-	3
25	-	-	8
30	8	-2	-
42	-	-	-22
48	-4	-3	-
60	-	-	6
69	-0.9	3	-
76	-	-	2
107	-	-	9
111	-0.9	4	-
136	-	-	2
140	-0.6	-3	-
181	-	-	3
185	-2	-2	-
227	-	-	3
232	+4	-0.2	-

[a] Inv. conc.; $R^2 = 0.991$.

[b] Power; $R^2 = 0.967$.

[c] Ln; $R^2 = 0.947$.

[d] Not collected.

[e] Data point not used in this analysis.

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APPENDIX A

INITIAL FEASIBILITY STUDY FOR AN ALVEOLAR SPIROMETER

RTI/140/01 April, 1989

VOC BREATH MEASUREMENT STUDY: ALVEOLAR BREATH METHOD

FINAL REPORT

by

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RTI/140/01 April, 1989

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SECTION 1
INTRODUCTION AND BACKGROUND

For nearly a decade, the U.S. EPA has been conducting studies of personal exposure to volatile organic compounds (VOCs) [1-3]. Participants in these studies have also provided breath samples which have confirmed actual exposure. For a few chemicals, e.g., 1,1,1-trichloroethane, trichloroethylene, tetrachloroethylene, p-dichlorobenzene, m,p-xylenes and ethylbenzene, correlations have been demonstrated between a person's activity, his/her personal exposure and breath levels [1]. Consequently, two general questions have arisen: (a) what are the common personal activities which may lead to elevated VOC exposure, and (b) can breath measurements provide a quantitative measurement of VOC exposure?

The collections of exhaled air for the determination of levels of organics in the studies mentioned above were made using a dual Tedlar bag spirometer. This device consists of a 40 L Tedlar bag, which holds clean, humidified, inhale air, connected through a mouthpiece assembly containing unidirectional flow valves, to a 40 L Tedlar bag which collects the whole breath provided by the subject. During sample collection, the subject draws air through the inhale bag and exhales into the Tedlar exhale bag through the one-way, Tedlar flap valve. Whole breath from this bag is then pumped out through a Tenax cartridge, which adsorbs the organic compounds present in the sample, for later analysis.

Except for demonstrating actual exposure through breath monitoring, little is known concerning personal activities and sources of VOCs which are responsible for exposure. Recently, a study was conducted in Northern New Jersey to examine the impact of activities such as dry cleaning clothes, smoking, home renovations, driving a car into an attached garage and use of room deodorizers on VOC levels in personal and indoor air [4]. Results from this study indicate that some VOC levels become elevated in some cases during these activities. In many cases, however, elevated levels of VOCs were observed which could not be explained entirely by the activities described above. Further research is needed to establish plausible links between sources and elevation of VOCs.

An interesting corollary question is - can breath measurements predict the VOC exposure level? The ability to use breath measurement data in lieu of personal monitoring would circumvent the participant burden experienced with personal monitoring and provide an alternative to blood collection and analysis, an invasive technique, for determining body burden. Currently employed models, however, which relate breath to the immediate periods of exposure are imprecise or need to be validated. The VOC residence time in the body is not well described in the literature for non-occupational situations, a parameter which is important in perfecting prediction models.

To address the above issues, research on breath monitoring techniques and breath monitoring during selected exposure situations was undertaken. The first two phases of this effort have been recently completed. First, a VOC canister based breath sampling method was validated. The addition of a canister technique to the spirometer method for breath sampling has expanded the spectrum of VOCs which may be collected and anlayzed from breath, specifically for VOCs with high vapor pressures and low breakthrough volumes on Tenax GC.

Secondly, a VOC exposure-breath montioring study in a clean-air chamber was conducted to produce high exposure to VOCs during usage of selected consumer products. This study provided an opportunity to (a) evaluate the canister based sampling method for breath, (b) compare blood-breath measurements, (c) calculate residence times for VOCs, and (d) demonstrate that some personal activities may lead to elevated VOCs in breath. Participants underwent presumed exposure, followed by post-exposure breath sampling over an extended period of time (greater than 8 hours). Results of this study indicate a successful accomplishment of the objectives [5] for some of the chemicals.

The chamber study, however, was only a first step in achieving these objectives, since several chemicals (e.g. dichloromethane, chloroform, vinylidene chloride, n-octane, n-decane, n-dodecane, etc.) were not sufficiently elevated to allow either a comparison of blood-breath levels, or a demonstration of the canister's ability to collect and preserve these chemicals from breath.

In addition, the desire to collect breath samples more rapidly and to use these to define early phase decay, requires the development of methodology for collection of alveolar air. The development of such a methodology is the subject of this report.

The device developed during the project is based on a simple open tube. Breath exhaled from the study participant is allowed to enter a Teflon open tube, rather than a Tedlar bag through a one-way valve where it is stored until the next exhalation. The breath is sampled into a canister through a sampling port just downstream of the exhale valve, i.e., breath is drawn from the tube into the canister. Because the last portion of breath to be exhaled is alveolar air, all of the breath collected after the initial passage of the deadspace air until the next exhalation is alveolar air. It is this alveolar air which has the highest levels of any compound which partitions from the blood into the alveolar sac and, hence, would be reflective of environmental exposure. A device of this sort will allow the rapid collection (in approximately one minute) of the breath so that detailed kinetic information regarding the elimination of the compound from the body can be obtained. This collection time compares favorably to the spirometer system, currently in use, where sample collection can take upwards of 15 minutes and limit the number of data point for a given study.

The ability to collect breath samples quickly is only one of the goals of this development effort. Another goal is that the device be miniaturized so that field transport is not a problem. The ability to bring the sampling device to the subject with a minimal effort will allow the acquisition of samples representing the earliest eliminations and provide the best resolution for characterization of the decay process. The other goal, which is consistent with the miniaturization, is that of simplicity. Although simplicity is not a prerequisite for usefulness, a device which is difficult to use and requires a fair degree of knowledge and skill will not be widely utilized and this will limit its impact. Throughout the development of this device, ease of use was always a main consideration.

Several experiments or groups of experiments were designed to answer questions critical to the optimal performance of the device. Starting from the concept of a breath collection system based on an open tube, the dimensions of this tube were studied with regard to the preservation of a high level CO_2 "plug" as determined by monitoring the CO_2 level with a mass spectrometer (MS). The effect of sample collection flow rate into a canister was also studied here. Second, having decided upon the optimal dimensions of the tubing, the fraction alveolar air collected using continuous sampling into a canister was studied. Several breathing rates and breath volumes were studied. Third, the precision of replicate breath samples was studied as a function of sample collection time. Finally, the recoveries of organic compounds through the newly-designed exhale valve were determined. Each of these considerations is presented, in turn, in the following sections.

SECTION 2
CONCLUSIONS

Work performed under this task has shown that a miniaturized breath sampling device is feasible and quite simple to operate. The device collects a portion of exhaled breath from a 0.5 inch internal diameter open tube through a sampling port, located very near the place where the breath enters the tube, into a 2 L canister. Unidirectional flow valves control air flow as in the current spirometer. Carbon dioxide measurements showed that greater than 95% of the breath sampled continuously into a canister at 3 L/minute is alveolar in origin. When breath was sampled continuously into a canister at a flow of 1.5 L/minute, this value increased to 97+%. The ability to sample and collect such high fractions of alveolar air without the need to open and close a valve to the canister greatly simplified the method. Using the described device and 2 L canisters with inlet flow rates of 1.5 L/minute, it was shown that sufficient sample for analysis could be collected in one minute. The collection of breath volumes larger than the anticipated alveolar volumes is unlikely under these conditions. In addition, when sampling sequential breaths from a single subject, the device can be ready to collect the next sample in only a minute or two. Such a short sampling time when combined with a rapid exchange of the sampling canister will allow for detailed descriptions of decay kinetics. The concentrations of organic compounds in the breath collected with the new device were higher than are those in whole breath, as in the currently used spirometer. Recoveries of a variety of organic compounds at both 4.4 and 36 $\mu g/m^3$ were found to average 101% and 96%, respectively, with no indications of cross-contamination between streams with the different concentrations of organic compounds.

SECTION 3
RECOMMENDATIONS

Given the success of phase one of this work (proof of concept and preliminary validation), field comparisons to the current spirometer and further validation studies are recommended. The validation studies should include an expansion of the target chemical list to include other compounds of interest and the utilization of 1 L canisters for sample collection. The smaller canister volume will contribute to the compact nature of the device as well as reduce the bulk of the canister samples to be shipped to the laboratory for analysis. Furthermore, the device should be refined to optimize the compact nature and resultant packaging to maximize portability while at all times keeping simplicity as a prime concern. Finally, the device as used here required a source of clean air for inhalation; alternatives should be investigated. For example, a small filter and battery powered pump might allow the use of ambient air rather than having to depend on an inhale bag filled at a location other than the exposure site. Such alternatives will optimize the portability and utility of the device.

SECTION 4
EXPERIMENTAL

EFFECT OF TUBE DIMENSION AND SAMPLING FLOW RATE ON PRESERVATION OF ALVEOLAR AIR PLUG

The first step in the development of the alveolar air sampling device based on sampling from an open tube is to consider the effects of gaseous diffusion and sampling rate on the preservation of the "plug" of exhaled, alveolar air. Once the tube is filled with exhaled breath, diffusion of both the alveolar air (high carbon dioxide level) and deadspace air (low carbon dioxide level) begins with the result that the CO_2 concentration gradient between the two regions becomes more shallow with time. The optimal geometric configuration will minimize the diffusion and maintain a distinct CO_2 concentration "step change." In this regard, a small diameter tube should better maintain the alveolar air plug than a larger diameter tube which allows for more diffusion because of its larger cross sectional area.

The rate at which the exhaled, alveolar air is sampled is also important; the optimal sampling rate is expected to be dependent on the internal diameter of the tube. In this case, laminar flow is an issue and should cause more profile distortion in narrow tubes than in wide tubes and at fast flow rates compared to slow flow rates. For the experiments described here, we used both 0.5 and 1.0 inch i.d. Teflon tubing to hold the exhaled breath, and sampling flow rates of 1.2, 2.3, and 3.3 L/minute. A laboratory worker served as the source of the exhaled breath. Carbon dioxide levels were monitored with a mass spectrometer.

The device used in these experiments is shown, in a general sense, in Figure A-1 and consisted of a custom Teflon mouthpiece connected through a 1 inch ball valve to the custom Teflon sampling port/tubing adapter, the Teflon tubing to contain the exhaled air, a Precision Dynamics three-way solenoid valve, a Tylan flow meter, and a Thomas double diaphram pump connected through a 2 L ballast and a needle valve to provide the desired flow rate. Two tubing adapters were used, one for 0.5 inch tubing and one

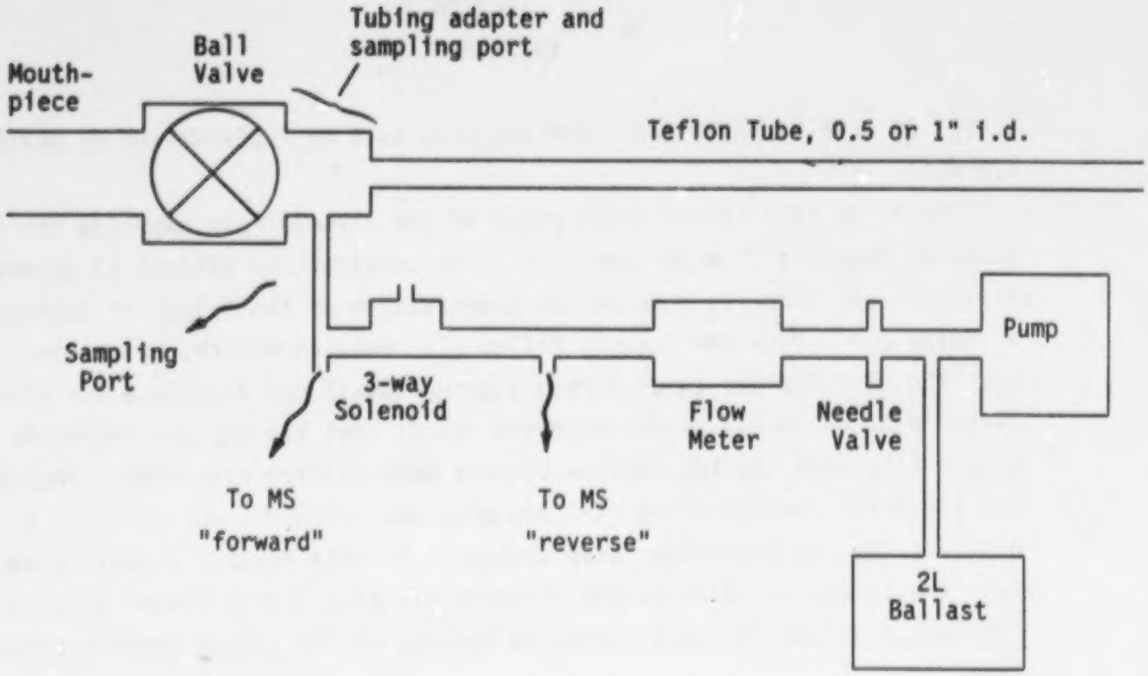
Tubing adapter and sampling port
Ball Valve
Mouth-piece
Teflon Tube, 0.5 or 1" i.d.
Sampling Port
3-way Solenoid
Flow Meter
Needle Valve
Pump
To MS "forward"
To MS "reverse"
2L Ballast

Figure A-1. Schematic diagram of the device used to study effects of tube diameter and sampling flow rate.

for 1 inch tubing. They were identical up to the point of decreasing diameter for connection to the Teflon tubing. A small fraction of air was sampled continuously for CO_2 using an LKB mass specrometer connected, through the direct probe inlet, to the device via a 170 cm section of 50 μm i.d. fused silica tubing (dimensions of which were chosen to maintain a vacuum of 3 x 10^{-5} torr in the mass spectrometer). The sweep time of the fused silica tube transfer line was 6 seconds. That is, there was a delay of six seconds after CO_2 passed the end of the tube before an increased level of CO_2 was measured in the mass spectrometer. The actual configuration was dependent on the experiment in progress and will be described at the appropriate time.

In order to describe the degree to which the alveolar profile is preserved, the alveolar air profile into the device must first be characterized. In this case, the silica transfer line was inserted into the sampling port until it was flush with the interior flow path of the adapter fitting. The three way solenoid was used to isolate the pumping system from the collection system, i.e., essentially a no sampling situation. The breath donor breathed repeatedly (inhalation through nose, exhalation through mouth) into the device without removing his mouth from the mouthpiece while the mass spectrometer was set to continuously monitor $\underline{m}/\underline{z}$ 44, the parent ion for CO_2. Each breath profile was studied closely and the slope (intensity change per scan) of the linear portion of the CO_2 increase was determined. The value obtained for each tube diameter was termed "Input (forward) slope."

The next experiment studied how well the input profile was preserved by the device as a function of both sampling flow rate and tube diameter. For this experiment, the fused silica line was moved to the port downstream of the three way solenoid valve, as shown in Figure 4-1, and the flow rate was set using the needle valve as the pump drew in air through the unconnected leg of the solenoid. The "forward" port was closed. After the subject exhaled, he simultaneously closed the ball valve and activated the solenoid so that air was now pumped from the 0.5 or 1.0 inch Teflon tube. In this case, a rapid increase in the CO_2 level was observed as the last portion of the alveolar air exhaled was drawn past the silica MS inlet tube. This elevated CO_2 level was observed until the first portion exhaled was drawn past the inlet to the MS whereupon the CO_2 level returned to baseline. Four breaths were studied in each case.

MODE OF SAMPLING

The determination of the fraction of alveolar air collected was accomplished in the following manner. The participant was asked to breathe repeatedly into the device (Figure 4-1), by inhaling through the nose and exhaling through the mouth into the mouthpiece. Breathing rate was consciously controlled by the subject with the aid of audible timers. In addition, the participant was asked to control breath volume to the best of her ability. The CO_2 levels were monitored with the mass spectrometer with the fused silica MS inlet connected to the port labeled "Reverse" while the pump drew air from the device at two flow rates. Before each experiment, i.e., each breathing rate, volume, and sampling flow, several single breaths were given and sampling was started after the exhalation. The sampling was continued until the CO_2 level returned to baseline. Through a knowledge of the sampling flow rate, the apparent alveolar volumes were calculated.

After it was clear that the participant was breathing appropriately for a given experiment, repeated breaths were given and sampling was started after the first breath and continued for 1.5 - 2 minutes. The type of information obtained from the mass spectrometer is shown in Figure 4-2 which shows the result of slow and shallow breathing with continuous (3 L/-minute sampling. The total area (positive) under the curve between the user-defined points (indicated by arrows in Figure A-2) was determined using the MS data system software as were the areas of the "dips" corresponding to the passage of deadspace air (negative areas). The absolute value of the sum of all of the dips was added to the total area and divided into the absolute area sum of the dips. This value is the fraction of the area corresponding to the contribution of deadspace air. This value was then subtracted from 1 to obtain the fraction of alveolar air sampled.

DETERMINATION OF ALVEOLAR CO_2 CONCENTRATION AND ITS DILUTION IN WHOLE BREATH

The purpose of this study was two-fold. First, the concentration of CO_2 in alveolar air was needed to allow the preparation of standards for task 3 of this project as well as for the later validation experiments in

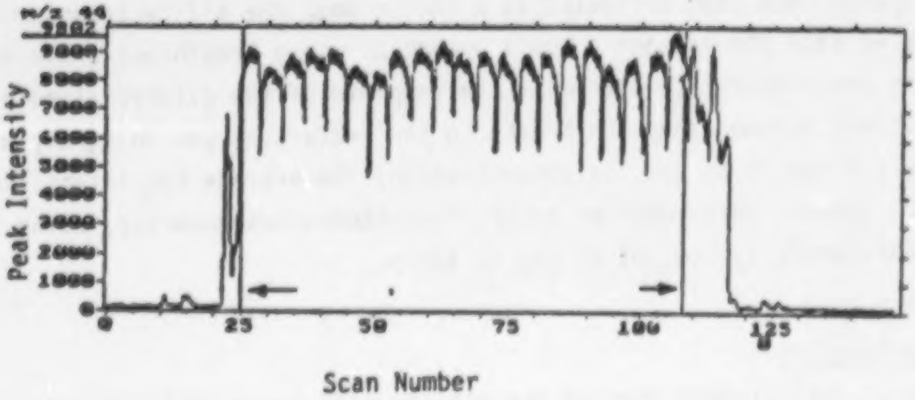

Figure A-2. CO_2 profile with continuous sampling.

the current task. Second, the CO_2 concentration in whole breath needed to be determined so that claims to the superiority of the open tube sampling device could be justified.

For this experiment, five different people provided at least three breaths into the open tube device, with the fused silica inlet to the mass spectrometer in the same position as for the characterization of the forward profile. The plateau ion current intensity of $\underline{m}/\underline{z}$ 44 for each breath was determined, i.e., the ion current given by room air was subtracted, and the values were averaged. Breaths from two of the participants were also collected in a Tedlar bag; the silica transfer line was placed into the bag and a small amount of whole breath was drawn into the mass spectrometer to determine the response of the diluted alveolar air. It was assumed that the breath in the Tedlar bag was uniformly mixed. For the estimation of the CO_2 concentration, the average ion intensities for each subject were compared to the ion intensities observed, using the same measurement system, of 6% CO_2 in air.

PRECISION STUDIES

Syringe Sampling

One of the intended uses of the miniaturized breath collection device is for kinetic studies to determine the elimination half lives of organic compounds from the body. Because the early phase of elimination can be very rapid, the ability to collect and analyze single breaths would be an advantage. Towards this end, we investigated the constancy of the levels of both CO_2 and an organic (toluene) in breath using 100 mL gas syringes (Precision Sampling Corp.) for sample collection from the new device. In addition, a Tedlar bag was filled with breath and air was withdrawn into a canister which was analyzed to determine the dilution of the organic in whole breath.

The device used for this experiment is shown in Figure A-3 and is basically one-half of the spirometer currently in use. The exhalation part of the spirometer was modified by attaching the newly designed collection system to the outlet of the mouthpiece union through a 1 inch ball valve which was used to isolate the Teflon tube/sampling part from the mouthpiece for the single breath experiments. During the experiment, study participant, who had been working with toluene, breathed normally from the

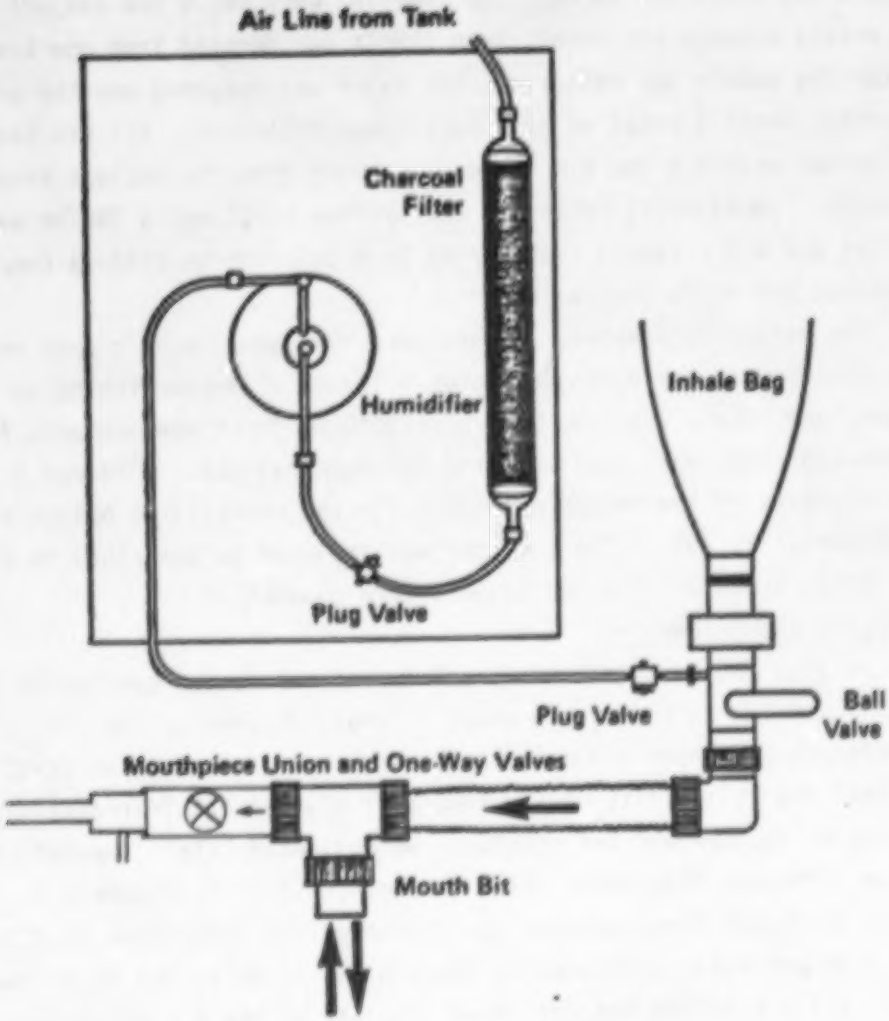
Air Line from Tank
Charcoal Filter
Humidifier
Plug Valve
Inhale Bag
Plug Valve
Ball Valve
Mouthpiece Union and One-Way Valves
Mouth Bit

Figure A-3. Device used to test precision based on syringe samples.

inhale bag and, after an exhalation, closed the ball valve and a 100 mL sample was withdrawn through the sampling port while the subject continued to exhale through his nose. Each sample was derived from one breath. After the sample was collected, the valve was reopened and the process was repeated until a total of six samples was collected. All six samples were collected within a few minutes during which time the subject exhaled 37 breaths. Immediately following the syringe sampling, a Tedlar bag was also filled and a 6 L sample transferred to a canister to allow a comparison of alveolar and whole breath levels.

The collected samples were analyzed the same day by slowly expelling the contents of the syringe through a length of Nafion tubing to remove water, and into a cryotrap held at -150°C to focus the contents for gas chromatographic/mass spectrometric (GC/MS) analysis. This was a modification of the method developed for the analysis of breath samples from canisters [5]. The canister was analyzed as described in reference 5. Both carbon dioxide and toluene were quantified.

Canister-Based Sampling

We also chose to test the precision of the system configured in a manner similar to the way in which it would be used in the field, i.e., continuous breathing and continuous sampling into a 2 L canister. In order to test the reliability of the sample if the number of breaths integrated during collection was not constant, we collected triplicate canisters at three different flow rates using the device shown in Figure A-4. Using three different flow controlling orifice giving flow rates of 2.31, 1.63, and 0.99 L/minute, and sampling times of 39 s, 55 s, and 91 s, respectively, a 1.5 L volume was delivered into all of the 2 L canisters. This volume was chosen to allow replicate GC/MS analyses of the same sample; the method requires that the canister be approximately 75% full for reliable replicate analyses. The use of 2 L canisters makes this situaiton possible in a minimal time and will allow for kinetic studies of organics in breath.

The experiment was performed as follows. First, the volunteer participant worked with toluene and dichloromethane for 30 minutes and then waited for 45 minutes to allow the initial decay to occur. At the sampling device, the participant took five breaths from the clean air inhale bag before beginning the three collections at the highest flow rate. Each

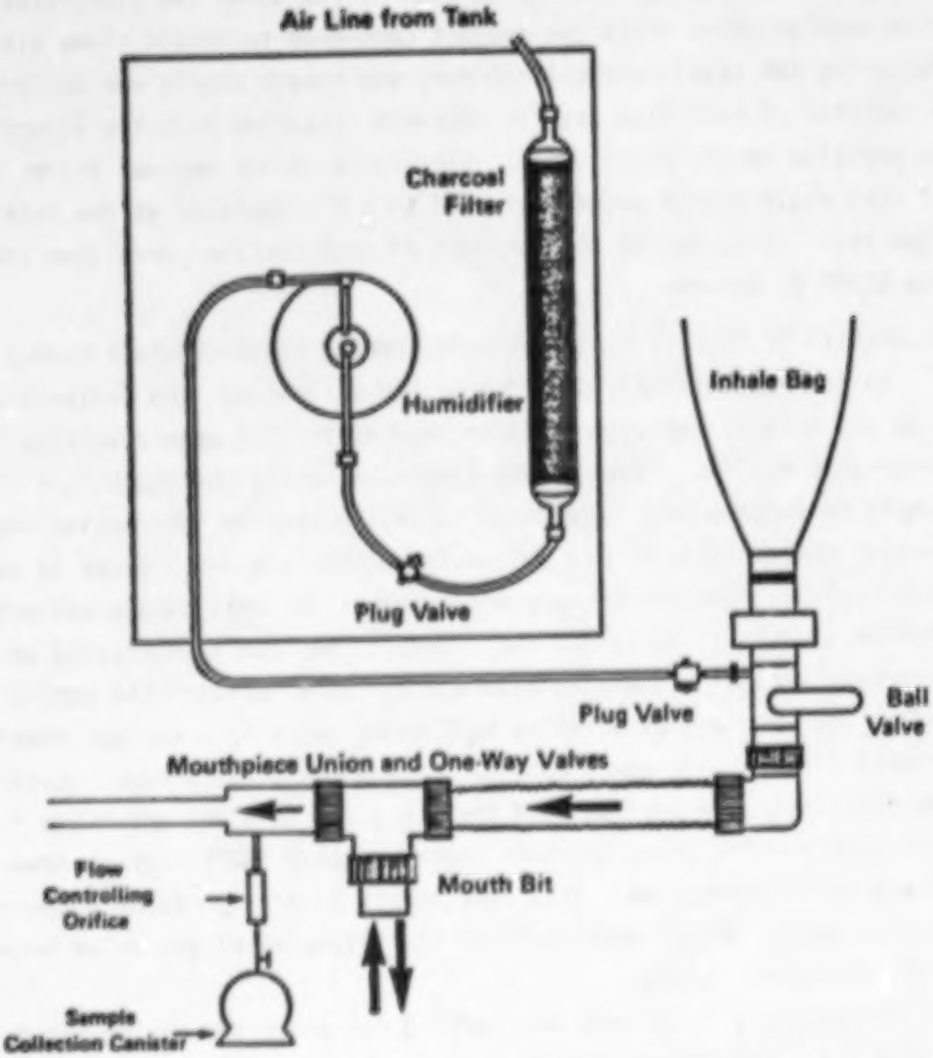
Air Line from Tank
Charcoal Filter
Humidifier
Plug Valve
Inhale Bag
Plug Valve
Ball Valve
Mouthpiece Union and One-Way Valves
Flow Controlling Orifice
Mouth Bit
Sample Collection Canister

Figure A-4. Device as configured for precision study based on canister sample.

collection was begun at the end of an exhalation for greatest reproducibility. The three collections at each of the other two flow rates were then made as above while the subject continued to inhale clean air. following the triplicate collections, one breath sample was collected into a canister at each flow rate in sequence, starting with the slowest flow to be opposite to the order above. Finally, a Tedlar bag was filled and 1.5 L of this whole breath was transferred to a 2 L canister at the intermediate flow rate. Aliquots of the contents of each canister were then analyzed via GC/MS as before.

RECOVERIES OF ORGANIC TEST COMPOUNDS THROUGH NEWLY-DESIGNED EXHALE VALVE

In the conventional, dual Tedlar bag spirometer, the Tedlar flap valves (one way valves) can often fail to seal or fail to open resulting in an inoperable device. These valves cannot be easily checked before starting sample collection and, once found to be the problem, correction requires partial dissassembly of the spirometer mouthpiece and a delay in sample acquisition. This can be very inconvenient if rapid sample collection for kinetic studies is an issue. As a result, we have investigated an alternate design as shown in Figure A-5. It is constructed entirely of Teflon and operates by a Teflon ball which seats in a conical opening and permits flow in only one direction. Stainless steel screws, isolated from the flow path, are used to hold the top plate in place and allow for easy disassembly. The valve has been heated to over 100°C with no adverse effect on its operation. This last aspect is of importance because of the need to have a design which permits sterilization of the valve between different participants.

The recovery experiment was carried out using the device shown in Figure A-6. For several hours prior to the start of the experiment, the standard containing 4.8% CO_2 in air was allowed to bubble through the controlled temperature impingers to humidify the stream and to bring the CO_2 concentration in the water to equilibrium. After humidification, the gas stream passed by the outlet of a pressurized fortification canister, the flow from which was controlled by a Tylan flow controller, to receive known amounts of the target compounds (Table A-1) into the stream. After the gas stream was thoroughly mixed, part of it was sampled into a verification canister, to provide a reference for recovery calculations,

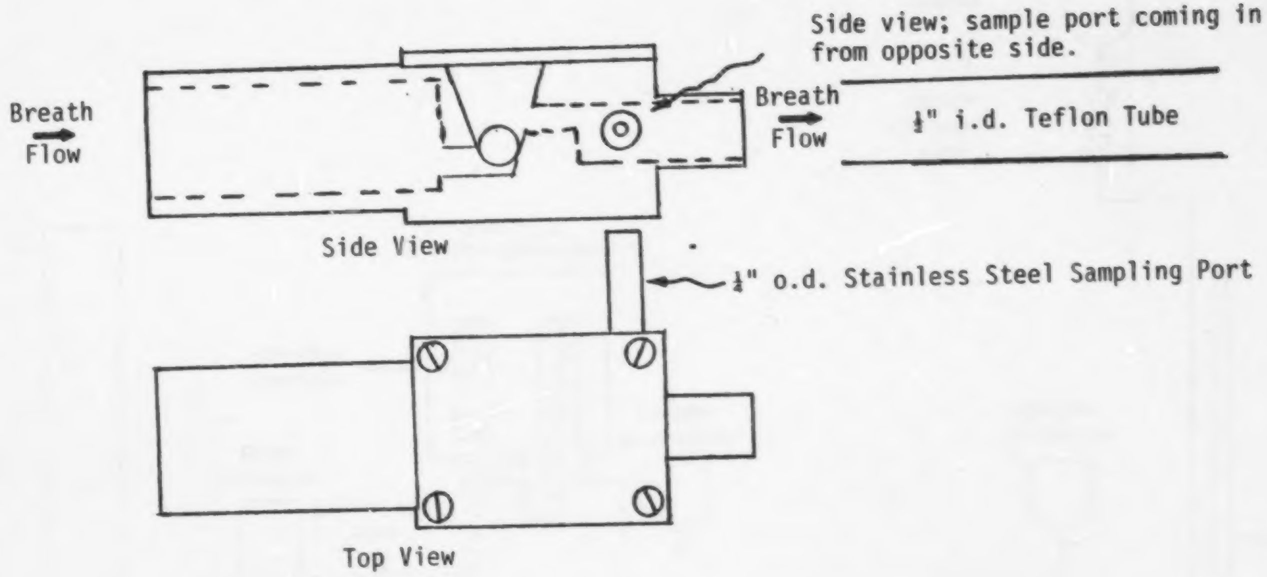
Breath
Flow
Side view; sample port coming in from opposite side.
Breath
Flow
¼" i.d. Teflon Tube
Side View
¼" o.d. Stainless Steel Sampling Port
Top View

Figure A-5. Exhale valve and sample port.

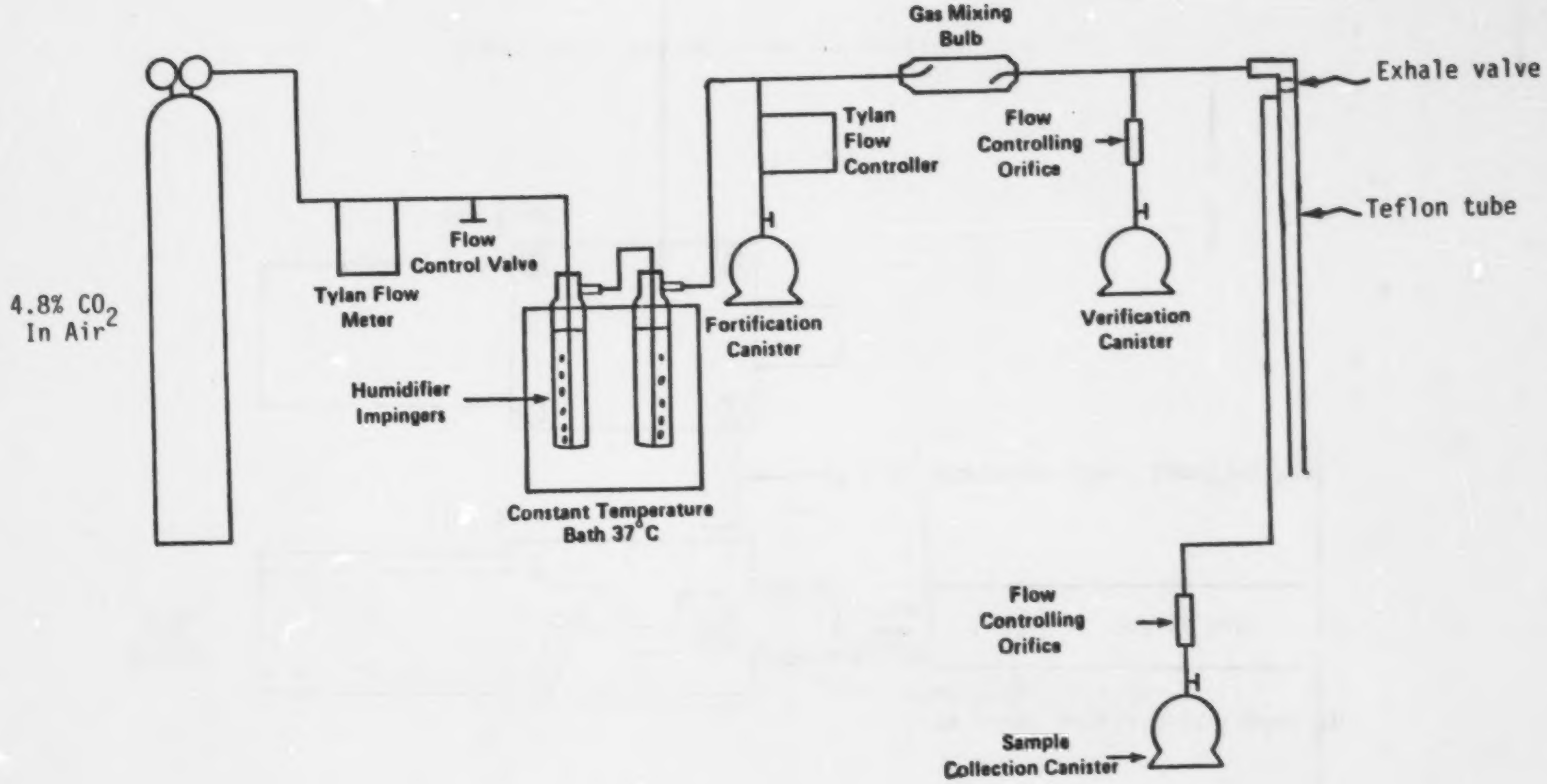
4.8% CO$_2$ In Air
Tylan Flow Meter
Flow Control Valve
Humidifier Impingers
Constant Temperature Bath 37°C
Fortification Canister
Tylan Flow Controller
Gas Mixing Bulb
Flow Controlling Orifice
Verification Canister
Exhale valve
Teflon tube
Flow Controlling Orifice
Sample Collection Canister

Figure A-6 Device used to generate synthetic breath for recovery studies.

TABLE A-1. CONCENTRATIONS OF TARGET COMPOUNDS IN THE PRIMARY STANDARD

Compound	Prim. Std. Conc. (ng/mL @ STP)
Vinyl chloride	39
Isopentane (2-methylbutane)	17
Vinylidene chloride	20
n-Pentane	17
Dichloromethane	21
2-Methylpentane	18
Chloroform	24
1,1,1-Trichloroethane	22
Carbon tetrachloride	17
Benzene	19
Trichloroethylene	24
n-Octane	19
Toluene	19
n-Nonane	19
Tetrachloroethylene	17
Ethylbenzene	19
p-Xylene	19
Styrene	20
o-Xylene	19
n-Decane	20

before passing through a 1 inch i.d. Teflon elbow which held the new exhale valve. The gas stream exiting the valve was collected in the sample canister. The sample canister was connected directly to the sampling port of the valve. The 2 L canisters were each filled for 60 seconds using the 21 ga. orifice which permitted a flow of 1.5 L/minute. All of the tubing and the mixing chamber up to the Teflon elbow were heated to 37°F. The gas flow into the new exhale valve was 5.45 L/minute as determined by the flow meter and verified downstream through periodic checks with a bubble flow meter during the course of the experiment.

The approximate concentration of each target compound in the primary standard was 20 ng/mL and was bled into the gas stream at a flow rate of 0, 1.15, or 9.45 mL/minute to yield final concentrations for each compound of approximately 0, 4,4, or 36.3 ng/L ($\mu g/m^3$). For convenience, these levels were termed zero, low, and high. These levels were introduced into the stream in the order zero, low, high, low, zero, high, and low to elucidate any potential problems with sample carry-over. The system was swept only briefly after changing the level before beginning the sampling. In a field application, this would be equivalent to having the participant provide a few breaths into the device prior to the collection of the sample. The canisters were analyzed as described in reference 5.

SECTION 5
RESULTS AND DISCUSSION

EFFECT OF TUBE DIAMETER AND SAMPLING FLOW RATE ON PRESERVATION OF ALVEOLAR AIR PLUG

Output from the mass spectrometer (MS) for the determination of the forward CO_2 profile in the 0.5 inch i.d. tube is shown in Figure A-7. The rapid increase in CO_2 level associated with the beginning of the alveolar air is clearly visible for each breath as are the "dips" which are associated with the passage of deadspace air over the silica tube with each new exhalation. The forward slope for both tube diameters are listed in Table A-2.

The rate at which the profile returned to baseline (Reverse CO_2 Slope) was indicative of the diffusion and mixing within the Teflon tube and the connecting tubing up to the point of the MS inlet. Because only the Teflon tube was changed at any given flow, changes in the slope observed upon changing tube diameters were caused by the Teflon tubing itself. An ideally preserved profile would have a slope equal to and opposite in sign from the input slope. The slopes compiled in Table A-2 clearly show that the profiles are better preserved using the smaller tube and fast sampling flow rates. As a result, it was decided that the 0.5 inch i.d. tube would be used to contain the exhaled breath. The data also show that a sampling flow as fast as possible should be used to preserve the profile. There are several considerations other than the profile preservation which needed to be considered before deciding on the "best" sampling flow; these are the subject of this section.

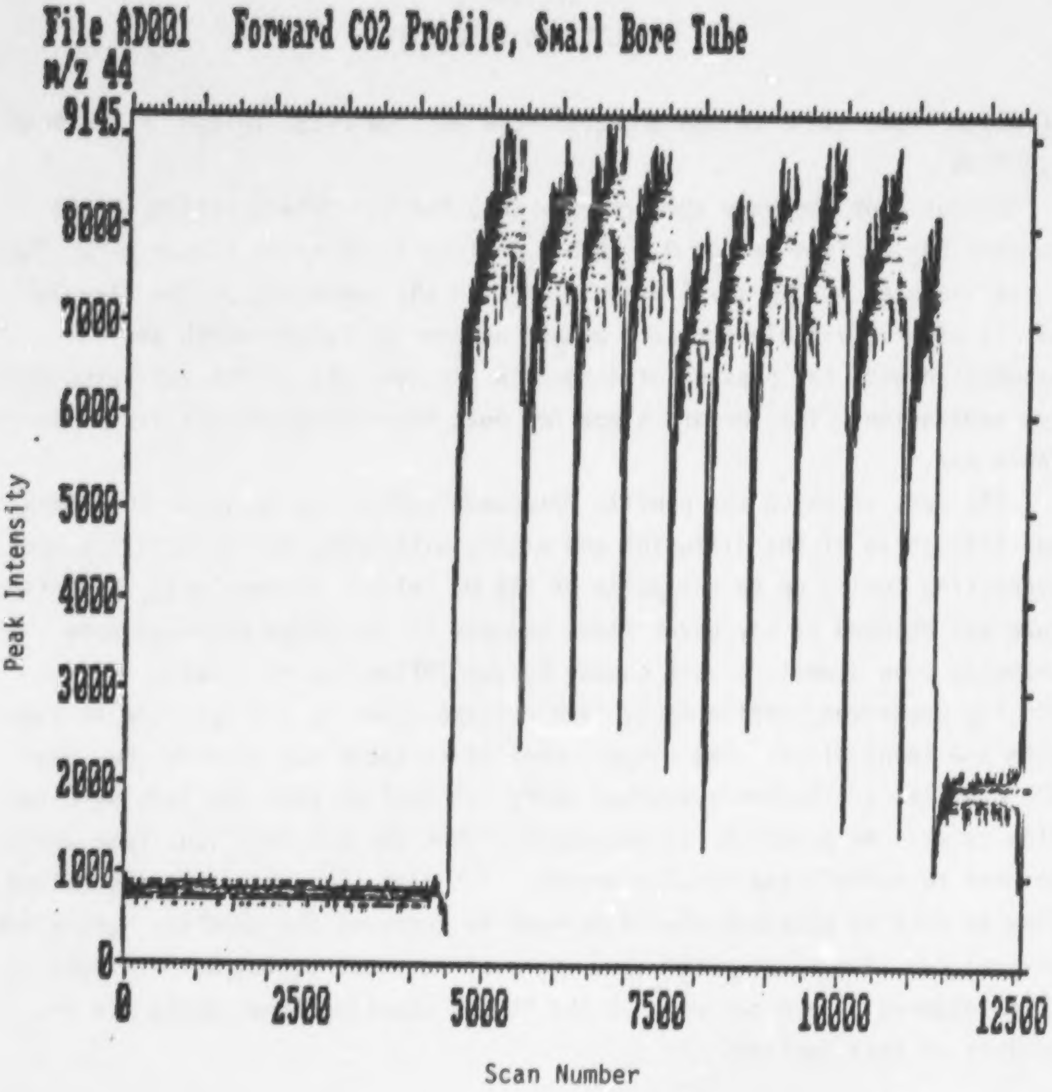

Figure A-7. Forward profile of m/z 44 (CO_2) with time and repetitive breathing.

TABLE A-2. EFFECT OF TUBE DIAMETER AND SAMPLING RATE ON ALVEOLAR AIR PLUG

Large (1 inch) Tube	Input (Forward) Slope = 132 (17% RSD) n = 10
Sampling Rate (L/Min)	Slope (% RSD) n = 4
1.2	-2.5 (23)
2.3	-4.4 (13)
3.2	-6.1 (22)
Small (0.5 inch) Tube	Input (Forward) Slope = 111.7 (19% RSD) n = 10
Sampling Rate (L/Min)	Slope (% RSD) n = 4
1.2	-13.6 (10)
2.3	-22.7 (5)
3.2	-31.3 (9)

MODE OF SAMPLING

Introduction

One of the goals of this project was to develop a device which samples exhaled breath and collects predominately alveolar air. Two modes of breath collection are possible with the device described in Section 4. The first is continuous sampling where breath is continuously drawn into the canister as the participant repeatedly exhales. This mode would be expected to collect some of the deadspace air in addition to the alveolar air. The second mode is the pulsed mode of sampling in which sampling is intermittent and is timed such that collection is allowed to occur only after the passage of the deadspace air for each breath. This mode would be expected to provide the highest fraction of alveolar air in the collected breath. The work described in this section deals with the determination of the fraction of alveolar air collected under a variety of breathing and sampling conditions using constant sampling.

At this point, the recall of some terms relevant to the physiology of respiration are needed. The "tidal volume" is the volume of air inspired and exspired with each normal breath and is equal to approximately 500 mL in the normal young adult male. Of this 500 mL, approximately 150 mL is termed "deadspace air" and is air which filled the nasal passages, the pharynx, the trachea, and the bronchi, and never entered the alveoli. The "inspiratory reserve volume" is the extra volume and is usually equal to approximately 3000 mL in the young adult male. The "expiratory reserve volume" is the amount of air that can be exhaled by forceful expiration after the end of the normal tidal expiration. This value is typically 1100 mL in the young adult male. The "residual volume" is the volume of air still remaining in the lungs after the most forceful expiration and this volume averages 1200 mL in the young adult male (6). All of these volumes are 20 - 25% lower in the female. With a "normal" breath, the fraction alveolar air in whole breath is expected to be 1 - (150/500) or 0.7. Although the deadspace volume remains constant, it is clear that if the participant draws on the reserve volumes, the resulting fraction of alveolar air would increase. This possibility was considered during the course of these experiments.

Results

Different types of breathing were investigated because of the variety of types found in actual sampling situations. A normal breathing rate is considered to be 12 breaths/minute yet there are extremes which could be encountered and, as a result, information on the fraction of alveolar air collected is required so that potential problem situations can be identified. The results of this series of experiments are summarized in Table A-3 from which several conclusions can be drawn. First, greater than 95% alveolar air was sampled in each situation and that at a flow rate of 1.5 L/minute, the fraction of alveolar air was 97+%. Thus, if the device was used to sample a person breathing at a rate of 15 breaths/minute and using a sampling flow of 1.5 L/minute, the alveolar volume would have to be below 100 mL for oversampling to occur. Such a small alveolar volume is unlikely in a healthy person and, even if such a small volume were encountered, the subject's rate naturally would be much faster to compensate for the small volume. Therefore, pulsed sampling would provide no real improvement and, given the goal of simplicity of the device design and operation, would actually be a hindrance because of the extra mechanical devices required.

The information about the apparent alveolar volumes indicates that when a person breathes into a device which does require some exertion, be it from this device or the currently used spirometer, some of the lung's reserve volume capacity is drawn upon. This is actually a benefit with either device as it makes more alveolar air available for collection with the open tube design and dilutes the deadspace air when sampling into a Tedlar bag with the current spirometer system.

The measured fraction was much higher than would be expected using the assumptions of an average volume for a young adult male of 500 mL/breath with 150 mL of that from deadspace air. In addition to the reserve volumes, as discussed above, we feel that discrimination against sampling the deadspace air arises from the air velocity during exhalation. The open tube device under study here samples at a constant rate and, if the breath is exhaled at a constant velocity, the fraction of alveolar air to be expected is approximately 85%, assuming 150 mL deadspace and 770 mL alveolar volume. From this, it is apparent that the exhalation velocity is not constant but rther the initial portion of the exhalation, which includes the deadspace air, passes over the sampling port much more quickly than the

TABLE A-3. FRACTION OF ALVEOLAR AIR SAMPLED AS A FUNCTION OF TYPE OF BREATHING, BREATHING RATE AND CONTINUOUS SAMPLING

					Measured Fraction of Alveolar Air			
Breathing Type	Breathing Rate	n	Avg. Alveolar Volume	%RSD	1.5 L/min	Number of Breaths Integrated	3.0 L/min	Number of Breaths Integrated
Fast and shallow	30/min	9	359 mL	28%	98.6%	9	95.8%	6
Normal	12/min	6	776 mL	2%	97.8%	17	97.0%	18
Slow and shallow	15/min	4	454 mL	6%	97.1%	21	97.4%	20
Long	6/min	5	770 mL	1%	97.9%	15	97.7%	24

alveolar air, with the result that it is under-sampled in proportion to its volume contribution. This is a major benefit to the open tube device because such velocity differences make no difference when whole breath is collected into a Tedlar bag.

DETERMINATION OF ALVEOLAR CO_2 CONCENTRATION

The results of this experiment are shown in Table A-4. From the data it can be seen that the average CO_2 concentration in alveolar air was 4.8%. The fraction of alveolar air in whole breath was determined to be 0.75 for one donor (female) and 0.88 for donor #2 (male). These values are greater than the literature fraction (350/500) of 0.7 and, again, is suggestive of some use of the reserve capacity [6].

PRECISION STUDIES

Syringe Sampling

The results of this experiment are shown in Table A-5. The variability of the toluene peak is quite large, particularly in view of the time duration of the experiment. Thirty seven breaths seems little enough time to result in a 30% decrease in the measured toluene level, especially since 40 minutes were allowed to elapse after exposure before starting the breath collections. That is, the initial, rapid decrease in the breath levels should have passed and the decay over the time of this experiment would have been expected to be much slower. In addition, the results of the analysis of the air captured in the canister from the Tedlar bag indicate that toluene was present at a level of 0.92 the alveolar value, which is greater than expected, and that the apparent level of CO_2 increased in whole breath. These inconsistencies suggested problems with the analytical method and our comparisons between the syringe samples and the canister sample. Because the syringe collection method had not been validated, its performance was questioned as was the dissimilar manner in which the syringe and canister samples were treated. As a result, we chose to repeat the experiment using canisters for the collections of all samples. Each was filled to the same extent so that analysis variations would be minimized. This work is described in the next section.

Canister-Based Sampling

The results of this experiment are presented in Table A-6. It is apparent that the levels of both dichloromethane and toluene decreased throughout the course of the experiment with the triplicate samplings.

TABLE A-4. DETERMINATION OF ALVEOLAR CO_2 CONCENTRATION AND DILUTION OF ALVEOLAR AIR IN WHOLE BREATH

Donor	Number of Breaths (n)	Average Intensity at Plateau of m/z 44 in Alveolar Air (%RSD)	CO_2 Conc. in Alveolar Air	Intensity of CO_2 in Whole Breath (Tedlar)	Fraction Alveolar Air in Whole Breath
1	3	27,128 (2%)	4.6%	20,380	0.75
2	3	32,200 (0.5%)	5.4%	27,720	0.86
3	7	29,200 (8%)	4.9%	-[a]	-[a]
4	3	24,551 (4%)	4.1%	-[a]	-[a]
5	3	29,341 (4%)	4.9%	-[a]	-[a]
6% CO_2	-	35,180 (n=1)	-[a]	-[a]	-[a]

Average Alveolar CO_2 Concentration = 4.8% (10% RSD)

[a] Not applicable.

TABLE A-5. RESULTS OF SYRINGE SAMPLING

Breath Number	CO_2 Area (m/z 44)	Toluene Peak Height (m/z 62)[a,b]
6	3.4×10^5	15,494
12	3.4×10^5	12,819
17	3.7×10^5	13,647
22	3.6×10^5	15,427
27	3.6×10^5	11,699
37	3.7×10^5	10,507
	$x = 3.6 \times 10^5$	$x = 13,332$
	%RSD = 3.5	%RSD = 13
Tedlar Bag Sample (100 mL)	3.7×10^5	12,265

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[a] m/z 62 was used because of saturation of m/z 91, a more intense ion.

[b] Peak height in arbitrary units.

TABLE A-6. CANISTER PRECISION STUDY RESULTS

Sampling Time	Time of Sample Collection After Start of Exp.	Average Peak Intensity[a] (%RSD)	
		Dichloromethane	Toluene
Triplicates			
39s	0-4:26	10953 (6.8)	21734 (10.1)
55s	6:32-10:35	8764 (1.8)	17885 (3.7)
91s	13:18-18:24	7694 (12)	14926 (4.4)
Sequential			
91s	21:43	6759	14794
55s[b]	24:42	6003	19125
55s (second analysis)		6100	19341
39s	26:52	6333	13434
Whole Breath (55s)	30:50-33:14	5525	10841

[a] Arbitrary units, n = 3.

[b] Canister suspected to be contaminated, values were excluded.

This continued decrease was seen in the sequentially collected canisters as well. The fact that this trend continued, despite a reversal in the sequence of flow rates, suggests that the measured concentration decreases were real and not dependent on sampling flow rate. If the average of the 39 s and 91 s sequential canister values from Table A-6 are taken for each compound, the relative standard error estimates (n=2) are 4.6% for dichloromethane and 6.8% for toluene. These lie well within the variabilities observed for the triplicate canisters (shown in Table A-6) and support our conclusions regarding the independence of measured concentration on the sampling flow rate. The sequential canister sample for 55 s was suspected to be contaminated as there were a great many chromatographic peaks containing $\underline{m}/\underline{z}$ = 57 (alkane). Canister samples collected at 91 s and 39 s showed no such contamination. The contents of this canister were also analyzed a second time and the same extraneous peaks were observed. Consequently, the values were not included in the calculations.

Upon comparison of the whole breath peak heights to those obtained by averaging the sequential alveolar samples at 39 and 91 seconds, the dilution observed in whole breath relative to alveolar air (fraction of alveolar air) was 0.84 for methylene chloride and 0.77 for toluene. These values compare well to those determined for CO_2 above. Although the CO_2 values were acquired from two donors, the organic dilutions were obtained from one person and the resulting different dilutions may be the result of differing solubilities of the organic compounds in the moist, mucous membranes of the airways. An increased solubility and later release ("off-gassing") could result in apparent lower dilution factors for more soluble compounds. These dilutions are also higher than the theoretical 0.7, supporting the hypothesis that some of the reserve capacity is used during sample donation.

RECOVERIES OF ORGANIC TEST COMPOUNDS THROUGH NEWLY-DESIGNED EXHALE VALVE

The results of the zero level canister analyses are shown in Table A-7, and indicate there was a problem with contamination of some of the canisters, especially the verification canister collected at 35:08 past time zero (t_0). The values shown represent raw peak height of the mass chromatograms. Low levels of benzene and dichloromethane are often seen as low

TABLE A-7. GC/MS PEAK HEIGHTS FROM ANALYSES OF ZERO (Z) LEVEL CANISTERS

Compound	Ion (m/z)	t_0 Zero Sample	t_0 Zero Verif.	35:08 Z Sample	35:08 Z Verif.
Isopentane	57	0	462	0	185
n-Pentane	57	0	5104	47	999
n-Octane	57	0	0	0	0
n-Nonane	57	0	0	0	44
n-Decane	57	55	0	44	88
Tetrachloroethylene	59	0	0	0	0
Trichloroethylene	60	0	0	0	51
Vinylidene chloride	61	0	0	0	0
1,1,1-Trichloroethane	61	0	0	0	135
Vinyl chloride	62	0	0	0	0
2-Methylpentane	71	0	0	0	0
Benzene	78	416	179	339	541
Carbon tetrachloride	82	0	0	0	0
Chloroform	83	0	49	0	2054
Dichloromethane	84	241	125	0	537
Toluene	91	0	0	0	210
Ethylbenzene	91	0	0	0	0
p-Xylene	91	0	0	0	76
o-Xylene	91	0	0	0	0
Styrene	104	0	0	0	0

level contaminants in the analytical system when sampling from a clean canister filled with alveolar air. This contamination reemphasizes the importance of knowing the history of the canisters to be used in a sampling effort and the importance of extensive background checks. These canisters had been used to sample stack gases.

The calculated recoveries ("sample" peak height/"verification" peak height) are summarized in Tables A-8 and A-9 for the low level and high level tests, respectively. For the low level recoveries, one of the three sample canisters was quite contaminated containing high levels of vinyl chloride, benzene, ethylbenzene, xylenes, and styrene. As a result, this collection was excluded from the summary table. Carbon tetrachloride was not found in one of the samples because of the low MS response typical for this compound, so the indicated recovery is derived from one analysis. The xylenes and styrene were excluded from the average recovery value because of the large variabilities which are consistent with low-level contamination, already known to be a problem. Overall, the recoveries are quite good and there was no evidence of sample carry-over. The high level recoveries showed much better overall precision, as would be expected. It is interesting to note that vinylidene chloride, 1,1,1-trichloroethane, vinyl chloride, benzene, carbon tetrachloride, chloroform, and dichloromethane all showed recoveries in the 79-88% range. The reason for this is not clear.

TABLE A-8. RECOVERIES OF TARGET COMPOUNDS AT LOW (4.4 NG/L) LEVEL

Compound	Average % Recovery	% RSD
Isopentane	95.9	7
n-Pentane	99.1	25
n-Octane	93.9	2
n-Nonane	82.6	20
n-Decane	97.0	28
Tetrachloroethylene	102.7	2
Trichloroethylene	107.1	2
Vinylidene chloride	103.6	5
1,1,1-Trichloroethane	96.6	3
Vinyl chloride	97.6	4
2-Methylpentane	98.5	10
Benzene	107.6	5
Carbon tetrachloride	97.6*	-[a]
Chloroform	99.7	8
Dichloromethane	89.8	6
Toluene	112.2	7
Ethylbenzene	133.5	2
p-Xylene	136.0*	8
o-Xylene	111.9*	35
Styrene	244.0*	46
Average Recovery	101.1% (Excluding "*")	
% RSD of Avg.	11%	

[a] This recovery determined from one value only.

TABLE A-9. RECOVERIES OF TARGET COMPOUNDS AT HIGH (36 NG/L) LEVEL

Compound	Average % Recovery	% RSD
Isopentane	97.2	1.3
n-Pentane	98.5	2.7
n-Octane	103.6	7.4
n-Nonane	102.1	3.0
n-Decane	104.0	4.7
Tetrachloroethylene	101.9	3.0
Trichloroethylene	104.5	4.5
Vinylidene chloride	88.8	15.0
1,1,1-Trichloroethane	92.7	11.0
Vinyl chloride	90.9	4.4
2-Methylpentane	92.2	1.0
Benzene	89.6	14.5
Carbon tetrachloride	88.3	9.3
Chloroform	88.5	15.5
Dichloromethane	87.1	11.0
Toluene	96.2	2.9
Ethylbenzene	99.3	1.0
p-Xylene	102.3	5.5
o-Xylene	103.4	4.3
Styrene	92.8	13.6
Average Recovery	96.2%	
% RSD of Avg.	6.4%	

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APPENDIX B

REFINEMENT, TESTING, AND CONSTRUCTION OF A A PORTABLE ALVEOLAR SPIROMETER

RTI/150/01/01F September 30, 1989

DEVELOPMENT OF AN ALVEOLAR SAMPLING DEVICE

DRAFT FINAL REPORT

by

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D. A. Whitaker, and E. D. Pellizzari

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Contract Number: 68-02-4544
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ABSTRACT

A portable spirometer, suitable for field use, and designed to sample primarily alveolar breath in under two minutes resulted from this research. Six devices were manufactured for use in breath sampling studies. Collection of breath samples into 1.8 L Summa polished canisters will allow for at least four or five replicate GC/MS analyses from each canister. Trial use of a prototype device demonstrated its applicability to the collection of organic compounds present in breath at concentrations ranging from low ppb to ppm levels. This suggests great potential for application to breath analysis in both ambient and occupational environments. The use of organic vapor respirator cartridges to filter inhalation air used for removed all of the test compounds except dichloromethane to levels below the quantitation limit (QL) of the analytical method. Detected dichloromethane levels were generally not much greater than the QL. It is not known if the detection of this compound represents emission from the filter or if it was background from the laboratory environment in which the analyses were performed. Dichloromethane was retained by the filter up to a volume of 320 L after which breakthrough was detected. Thus, for the compounds tested, each filter can be used to provide up to 320 L of clean air before replacement is required, two filters are used in each spiro- meter. Recoveries of test organic compounds from the device at the 5 ppb level ranged from 89 to 112% with the exceptions of n-dodecane and 4-phenylcyclohexene. At the 50 ppb level, recoveries ranged from 91 to 109% with the exceptions of n-dodecane and 4-phenylcyclohexene. The results indicated no significant problem from either adsorption or carryover at these levels.

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SECTION 1
INTRODUCTION AND BACKGROUND

Methods that determine the concentrations of volatile organic compounds (VOCs) in human breath as indicators of environmental exposure are attractive both because the sample collection procedure is noninvasive and because those compounds that can be measured in breath are indicative of actual exposure. Such measurements should better reflect body burden than the presumed exposure information derived from air measurements. Despite the potential of breath analysis for exposure evaluation, it is not routinely used for exposure monitoring. Two main factors have been identified as contributing to the limited use of breath sampling and analysis (1). First, data interpretation is difficult. The relationships between breath concentrations and exposure levels are not clear, especially for environments with fluctuating VOC concentrations. In addition, there is limited information on the magnitude, origin, and significance of individual variations in VOC concentrations. Second, reliable and simple field methods are rare. Without a simple method for routine application, the studies needed to address the exposure level/breath level correlations and other issues will not be forthcoming. How we have addressed the methodological aspects of breath collection to build a portable spirometer system is the subject of this report.

Work performed under EPA Contract 68-02-4544, WA 40, Tasks 1 and 3, demonstrated that the alveolar breath sampling device, partially developed during Task 1, is capable of collecting principally alveolar air into an evacuated canister in a short time, approximately one minute. This device was subsequently used in Task 3 to help define the elimination of VOCs from the body after exposure to microenvironments. Although the device developed and applied in Tasks 1 and 3 showed a great deal of promise, it still utilized aspects of the whole breath collection system. For example, both methods required the production and storage of clean, humidified air for inhalation. Zero grade compressed air was filtered through a charcoal bed and then humidified before storage in a 40 L Tedlar bag. Air was drawn from the bag as needed through the spirometer inhale valve (Tedlar flap valve). This approach provided clean air for inhalation but severely limited the portability of the device; all samples were collected in a van driven to the site.

This report documents modifications made to the alveolar sampling device and collection procedures used in Task 3 (microenvironmental exposure study). Primary consideration was given to portability and ease of use. Aspects of the device studied and described in this report are (1) the source of clean air for inhalation, (2) the choice of the smallest possible canister for the collection of breath samples, and (3) characterization of the recovery and carryover behavior of the complete device, less the inhale portion. The results of these experiments were used to design and build six portable, field sampling devices.

SECTION 2
CONCLUSIONS

This work resulted in a field portable, useable spirometer, that was designed to sample primarily alveolar breath in under two minutes. Six devices were manufactured for use in breath sampling studies. Collection of breath samples into 1.8 L Summary polished canisters will allow for at least four or five replicate GC/MS analyses from each canister. Trial use of a prototype device in Task II-40 of this contract demonstrated its applicability to the collection of organic compounds present in breath at concentrations ranging from low ppb to ppm levels. This suggests great potential for application to breath analysis in both ambient and occupational environments. The use of organic vapor respirator cartridges to filter the air used for inhalation provided removal of all of the test compounds except dichloromethane to levels below the QL of the analytical method. Detected dichloromethane levels were generally not much larger than the QL. It is not known if the detection of this compound represents emission from the filter or if it was background from the laboratory environment in which the analyses were performed. Dichloromethane was retained by the filter up to a volume of 320 L after which breakthrough was detected. Thus, for the compounds tested, each filter can be used to provide up to 320 L of clean air before replacement is required; two filters are used in each spirometer. Recoveries of test organic compounds from the device at the 5 ppb level ranged from 89 to 112% with the exceptions of _n_-dodecane and 4-phenylcyclohexene. At the 50 ppb level, recoveries ranged from 92 to 109% with the exceptions of _n_-dodecane and 4-phenylcyclohexene. The results indicated no significant problem from either adsorption or carryover at these levels.

SECTION 3
RECOMMENDATIONS

Based on the results of this research, the following recommendations can be made. First, a field trial of the complete portable spirometer is recommended. This trial should be designed to evaluate the ruggedness of the device, its ease of use, the sampling procedures employed, and the background obtained from the device in a variety of sampling situations. Second, a protocol for field use of the system should be written. Finally, it is recommended that an alternate collection method e.g., the use of Tenax sampling cartridges, be validated for compounds less volatile than p-dichlorobenzene.

SECTION 4
EXPERIMENTAL

SOURCES OF AIR FOR INHALATION

For maximum flexibility in a breath collection method, it is desirable that the collection of sample be possible at any location and not limited to any fixed site far removed from the exposure area. The source of clean air for inhalation was, therefore, one of the most important aspects of this effort. At the start of this work, several options were considered for a clean air source. They were:

1. Ambient air to be inhaled through carbon respirator cartridges,
2. Air to be inhaled from a stream of filtered (cleaned) air provided by a high volume pump,
3. Filtered air to be inhaled from a small reservoir that is continuously filled by a low flow rate pump,
4. Clean, compressed air to be inhaled through an on-demand valve,
5. Air to be inhaled from a reservoir continuously filled by a small tank of clean, compressed air, and,
6. Clean air to be inhaled from a large Tedlar bag filled at a remote location and brought to the sampling system as needed.

Although all of these options could supply clean air for inhalation, not all of the choices met the overall goals of miniaturization, portability, and simplicity. For example, any source that requires the use of a pump, reservoir, or tank of compressed air severely compromises the portable nature of the device. In addition, a high volume pump would either require electricity or a very large portable power supply that would, again, compromise the portability feature. Therefore, we chose first, to investigate the potential of carbon (charcoal) VOC respirator cartridges to provide the clean air for inhalation. These devices do not need an external power supply or other bulky accessories, and therefore have the advantages of portability, simplicity, relatively low cost, and small size. The experiments designed to test the suitability of these cartridges are described below. As will be seen, the results indicated that no other option needed to be examined.

The respiratory cartridge filter was tested to evaluate the following: (1) the VOC background of the respirator cartridge, (2) the effectiveness and duration of VOC removal during continuous filtration of air spiked at ~1 ppm and ~10 ppm, and (3) the effectiveness of trapping organics on the same cartridge when intermittent sampling at ~10 ppm was conducted over several days. This last experiment was designed to ascertain if potential migration of VOCs within the adsorbent bed during storage between sample collections could cause alterations in the volume of air that could be filtered effectively. Along with these considerations were the cost of replacing respirator cartridges and the number of samples that could be collected using a single respirator cartridge without compromising the quality of the results.

Filter Background

The VOC background of the potential inhalation system was addressed in a relatively simple experiment. A respirator cartridge (Survivair Chemical Cartridge for organic vapors, P/N 1001-00) was attached to a machined teflon pipe that also had two other parts: one for drawing air through the respirator cartridge and one to sample the filtered air. Each respirator cartridge was used to filter laboratory air at 2 L/min for 37 minutes. Air samples were collected into an evacuated, 2 L canisters starting at 0, 15 and 35 min after filtration began. An orifice rated at 1.6 L/min at full vacuum was used to sample the filtered air for 75 sec so the canister would be filled to a pressure close to atmospheric. Laboratory air and laboratory air collected in the teflon pipe without the respirator cartridge were also collected. This experiment was repeated three times.

The analyses of the canister samples were carried out using a gas chromatograph/mass spectrometer system (GC/MS) with a canister air sampling interface. The canister air sampling interface is essentially a cryofocussing device that traps organic vapors from an air sample as the air is pumped from the canister. A Nafion drying tube was used to dry the air sample before cryotrapping. A schematic of the entire analytical system is shown in Figure B-1. A more complete description of the system can be found elsewhere (2). GC/MS analysis parameters are shown in Table B-1.

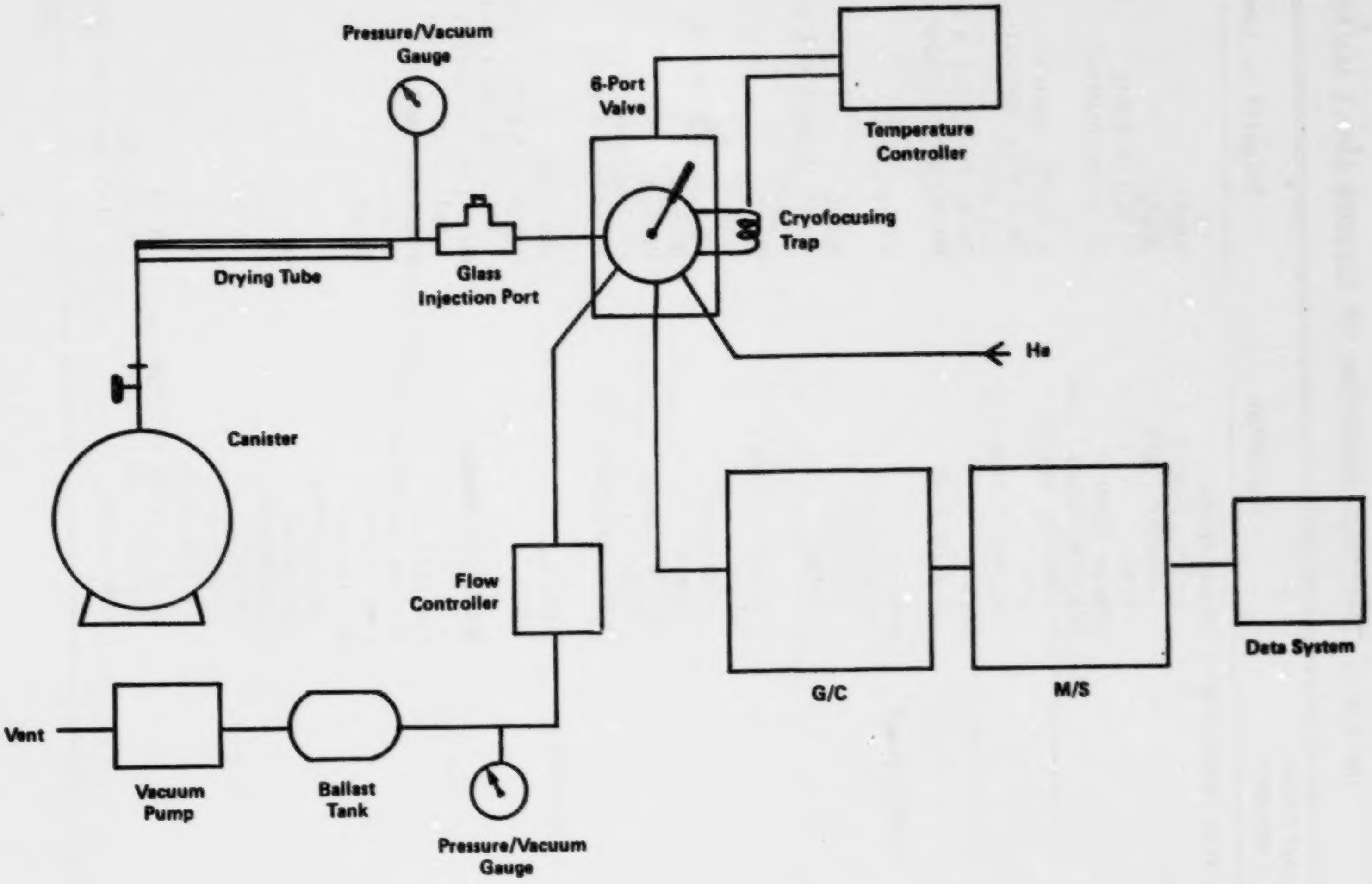
Pressure/Vacuum Gauge
6-Port Valve
Temperature Controller
Cryofocusing Trap
Drying Tube
Glass Injection Port
He
Canister
Flow Controller
G/C
M/S
Data System
Vent
Vacuum Pump
Ballast Tank
Pressure/Vacuum Gauge

Figure B-1. Schematic diagram of the analytical system used for the analysis of canister air or breath samples.

TABLE B-1. ANALYTICAL CONDITIONS FOR CANISTER SAMPLE ANALYSIS

Instrument Component	Parameter	Setpoint or Condition
Canister interface	Temperature:	
	valve, 6-port	200°C
	transfer lines	200°C
	trap	-150°C → 200°C
	Sample Flow:	20 sccm, nominal
	Trapping Time:	
	alveolar breath	3.0 min, nominal
	air	10.0 min, nominal
	external standard	2.5 min
	Dryer:	Perma Pure, 1.1 m x 1/8" o.d.
	drying flow	80 mL/min nitrogen
Gas Chromatograph	Model:	Varian 3700
	Temperature:	
	injector	200°C
	column	-20°C (0 min) @ 5°C/min → 200°C
	transfer line	200°C
	Column:	
	dimensions	30 m x 0.32 mm i.d.
	phase	DB-624
	Carrier Gas:	Helium
	flow	~2.7 mL/min
	head pressure	10 psig (70 KPa)
Mass Spectrometer	Model:	LKB 2091
	Type:	magnetic sector, single focusing low resolution
	Operation Modes:	multiple ion detection (MID), full scan
	Ionization:	electron impact
	Ionization Potential:	70 eV
	Trap Current:	50 μA
	Multiplier:	
	preamplifier	1
	setpoint	500
	Temperature:	
	inlet	160°C
	source	180°C
	Full Scan Mode:	
	accelerating voltage	3.5 kV
	magnetic sweep range	1 → 256 m/z
	scan speed	#2 (1.5 sec/scan cycle)

(continued)

TABLE B-1 (cont'd.)

Instrument Component	Parameter	Setpoint or Condition
Mass Spectrometer (continued)	MID Mode:	
	magnetic setpoint	57 m/z @ 3.5 kV
	ions: min. and max.	57, 104 m/z
	scan speed, cycle	1 scan/sec
	Reference Standard:	tris-(heptafluoropropyl)-s-triazine
	Vacuum:	~2 E-5 torr
Data Acquisition	Computer:	Tandy 3000 microcomputer
	MS Interface and Software:	Teknivent Vector/1 system
	Sampling Rate:	10000 samples/sec
	MID Mode:	
	sweep across ion	±0.2 m/z by 0.033 m/z
	sample time	1 mS
	samples averaged per ion	4 summed x 2 averagings
	A/D resolution	16 bit

For the analysis, the full scan mode of the GC/MS was used initially to verify the identity of any major constituents. Some samples were analyzed a second time without a drying tube in line to avoid losses of polar compounds of potential interest. Later experiments utilized the multiple ion detection mode (MID) for a selected list of hydrocarbons, aromatics and halogenated alkyl compounds. In this manner, maximum sensitivity would be available for target compounds.

Breakthrough Volumes of Target Compounds

Another test conducted on the respirator cartridge was designed to determine the breakthrough volume of a set of target compounds shown in Table B-2. Breatkthrough volume is defined as the filtration volume beyond which a VOC is no longer effectively removed from the gas stream. A knowledge of the breakthrough volumes is essential to determine how long a cartridge could be used in the spirometer before the cleanliness of the air for inhalation was compromised. The experiment provided levels of the compounds to the filter ranging from 550 $\mu g/m^3$ to 2800 $\mu g/m^3$ in ambient air. A liquid mixture of the analytes was prepared and placed into a reservoir through which nitrogen was bubbled. The effluent was then added to a stream of ambient air to provide the general levels of the compounds desired. This air mixture was delivered to a chamber constructed from a 12 L Pyrex™ bell jar on a polystyrene base covered with aluminum foil. A respirator cartridge was placed inside the chamber and connected to an external pump and to a sampling canister that collected the cleaned air. Another sampling canister collected chamber air that had not passed through the cartridge so that the levels of the compounds could be determined. Also, an additional port was used to vent excess spiked air from the chamber and prevent any pressure increase. These experiments were conducted at ambient temperature (~25°C).

The respirator cartridge filtered ~16 L/min of the spiked polluted air from the chamber. Samples of the filtered air were collected by 6 L canisters using an orifice rated at 2.3 L/min at full vacuum. Each sample was collected over 2 min. There were two levels of organics in air that were used to challenge the respirator cartridge, both of which were well above the levels generally encountered in environmental samples. This was carried out to probe the limits of the respirator cartridge applicablity.

TABLE B-2. LIST OF TARGET COMPOUNDS FOR EVALUATING THE EFFECTIVENESS OF RESPIRATOR CARTRIDGES

Isopentane
n-Pentane
2-Methylpentane
Benzene
Dichloromethane
Chloroform
Carbon tetrachloride
n-Butanol
n-Butyl acetate
Vinylidene chloride
1,1,1-Trichloroethane

For the lower level, filtered samples were collected beginning at 0, 82, 490, 980 and 2020 liters of total volume filtered. Unfiltered samples were collected beginning at 0 and 2020 liters of total volume. For the higher level, filtered samples were collected beginning at 0, 320, 650, 960 and 1290 liters of total volume filtered. Because of rapid depletion of the volatile analytes were rapidly depleted from the liquid mixture used in the bubbler, the solution was changed five times over the course of the experiment. Since some depletion occurs even with the solution change, the unfiltered samples were collected at the beginning and end of the third segment of the respirator cartridge loading to verify the levels used. For each level, the entire experiment required approximately 2 hours of essentially continuous filtering with intermittent sampling.

The analyses were carried out as for the previous experiment to determine the VOC background of the respirator. The analyses were accomplished using the MID mode of the GC/MS and the canister air samples were all dried through the tube drier prior to introduction into the instrument. In addition, the filtered and unfiltered air samples collected at 2020 L were analyzed without the tube drier to allow detection of n-butanol and n-butyl acetate. To expedite results for these two compounds, only the areas were reported as no previous standard was available. All other compounds were quantitated to provide concentrations.

Effect of Filter Storage and Reuse

Questions remained concerning the possibility of the reusing of the respirator filters and if storage in a relatively clean environment with intermittent use was possible. This would allow maximal use of the filters and result in cost reductions in materials required for breath sampling. Additionally, the higher levels of the organics would be of interest in case a breath sample from an individual in an occupational setting was desired. These data would help provide critical information regarding the range of applicablity with the respirator cartridges.

Essentially the same experiment as for breakthrough was performed except that the compound levels ranged from 0.5 to 23 mg/m^3 in air and samples were collected intermittently over a five day period. Approximately 320 liters of air were filtered each day over five days. Between days, the outlet of the respirator cartridge was capped and the cartridge was left in the chamber after the chamber was flushed out with ambient air. A slow nitrogen purge was provided overnight in the chamber to prevent possible contamination by laboratory air.

Each day before the start of the experiment, the solution of organic compounds used to introduce the test components into the chamber was replaced with fresh solution so that the level of each compound in the air stream would be essentially the same from day to day. Sample collection began at the start of each filtering cycle, 5 sec after filtering started. As before, the air flow was ~16 L/min and canister samples were collected at 2.3 L/min. Unfiltered samples were collected on the third day at the beginning and end of the filtering period to measure the concentration of organics delivered to the chamber. Due to the organic mixture in the bubbler, some more volatile compounds were depleted significantly during each day of the sample collection period.

The GC/MS analyses were carried out in the same manner as for the continuous filtering experiment.

CHOICE OF OPTIMAL CANISTER SIZE

Another parameter studied was the size of the canister used to collect the breath sample. The optimal canister should have a small volume so that it will fit easily into a portable sampling system yet should have a volume large enough to permit replication of the analysis. The volume should also be such that an adequate breath sample can be collected in 1-2 minutes so that kinetic studies for VOC elimination are possible. There are essentially two elements that define the limits of analyses from canisters: (1) trapping flow to the GC/MS cannot be quantitatively monitored when the vacuum in a canister exceeds 15" Hg, and (2) the trapped volume cannot exceed 60 mL for alveolar breath samples due to cryotrap freezing problems associated with high concentration of water and CO_2 in breath samples. Both of these elements interact to define a minimum canister volume. With regard to sample collection, the flow rate into a canister through a critical orifice employing a tube section drops once the canister vacuum is less than ~7.5" Hg. This element serves to under-represent VOC concentration for samples collected at later times and can be neglected here since a constant flow rate for a breath sample is not critical when the sample is collected over approximately 2 minutes. This would allow a canister to be filled close to ambient pressures, thus increasing the volume that can be analyzed from a given canister.

As mentioned before, another consideration of canister size is the ability of a given canister to permit replicate analyses of the same sample given the above constraints. In general, two analyses are the minimum needed, though three is a safer number to allow for instrumental failure or a slightly less than desired sample volume. Of course, greater numbers of analyses could be desired, but the physical size of the canister then becomes a problem for a portable spirometer system. Additionally, a large canister volume requires sampling flow rates too large for a slow breathing human subject, thus sampling ambient air along with the breath through the exhaust tube of the portable spirometer. Slower sample collection could be utilized but this would be at the expense of the time resolution desired. To provide a reasonable compromise, a minimum of three sample analyses from the same canister should be possible. Therefore the canisters must contain enough volume for: (1) residual nonanalyzable volume, or 1/2 of the canister volume, (2) the actual volume required per analysis step multiplied by three, and (3) the volumes consumed during an analysis which are not actually trapped multiplied by three.

As a first step, a simple experiment was devised to test the analytical capacity of 1 L air sampling canisters for breath samples. A spirometer was set up to provide the alveolar breath for the canister. Using a 0.99 L/min orifice (rated at full vacuum) over 1.0 min and an evacuated 1 L canister, the exhaled breath was collected leaving a vacuum in the canister of 3.8" Hg.

The canister was put through three analytical cycles of cryo-trapping. Each cycle included: (1) the initial flow surge from the canister as the valve is opened, but before the flow is regulated by the Tylan flow controller, (2) a 2.0 min x 20 standard cubic centimeters per minute (sccm) flush out period, (3) a 3.0 min x 20 sccm loading period, and (4) a 0.5 min x 20 sccm post-loading period. The measured volumes total 110 sccm, though somewhat more will have been expended per analysis cycle due to the initial surge. At each sample withdrawal, the remaining pressure in the canister was noted as was the ability of the system to maintain a flow of 20 sccm. As more sample is withdrawn from the canister, the vacuum increases which at some point will result in a drop in flow below 20 sccm. When the flow is not constant, quantification becomes difficult and unreliable.

ADDITIONAL RECOVERY STUDIES

The recoveries of several aliphatic, aromatic, and chlorinated hydrocarbons through the Teflon exhale valve were studied during WA 40, Task 1 of this contract and were found to average 101% and 96% for the test compounds at levels of 4.4 and 36 $\mu g/m^3$, respectively. This study tested the exhale valve only and was performed with a continuous flow of contaminated air through the system. What remained to be determined were the recoveries of a range of compounds from the system as it will be used in the field. That is, an investigation of the compound recoveries from air that has occupied the 0.5" Teflon sample collection tube was needed. This was accomplished by introducing a synthetic breath stream into the device in a manner that mimicked the inhale and exhale breath cycles. Adsorptive losses of compounds at low levels and carryover of compounds at higher levels were studied during this phase of the work and are described below.

The adsorptive loss and carryover experiments were quite similar so the same appratus was used for each. The system was essentially a synthetic breath generator with a (verification) canister to collect its effluent and two valves that were switched simultaneously so flow was directed either to the spirometer (exhalation) or out the side tube (inhalation). The apparatus is shown in Figure B-2. In addition, the spirometer had its own canister for sampling purposes.

Synthetic breath was generated by delivering air with 4.8% carbon dioxide to a flow control valve then to a humidifier. This humidified air was then mixed with a high concentration organic mixture (Table B-3) from the fortification canister at a known rate. Once the gas leaves the gas mixing bulb it is the final synthetic breath mixture spiked with known levels of organics.

Adsorption Studies

One of the major areas of interest was to characterize the adsorptive behavior of the spirometer system when used to collect a breath sample containing low levels of organics. Unsuspected losses would severely affect the accuracy of the analytical results. The approach taken here was to start with a clean and dry spirometer and to collect two sequential

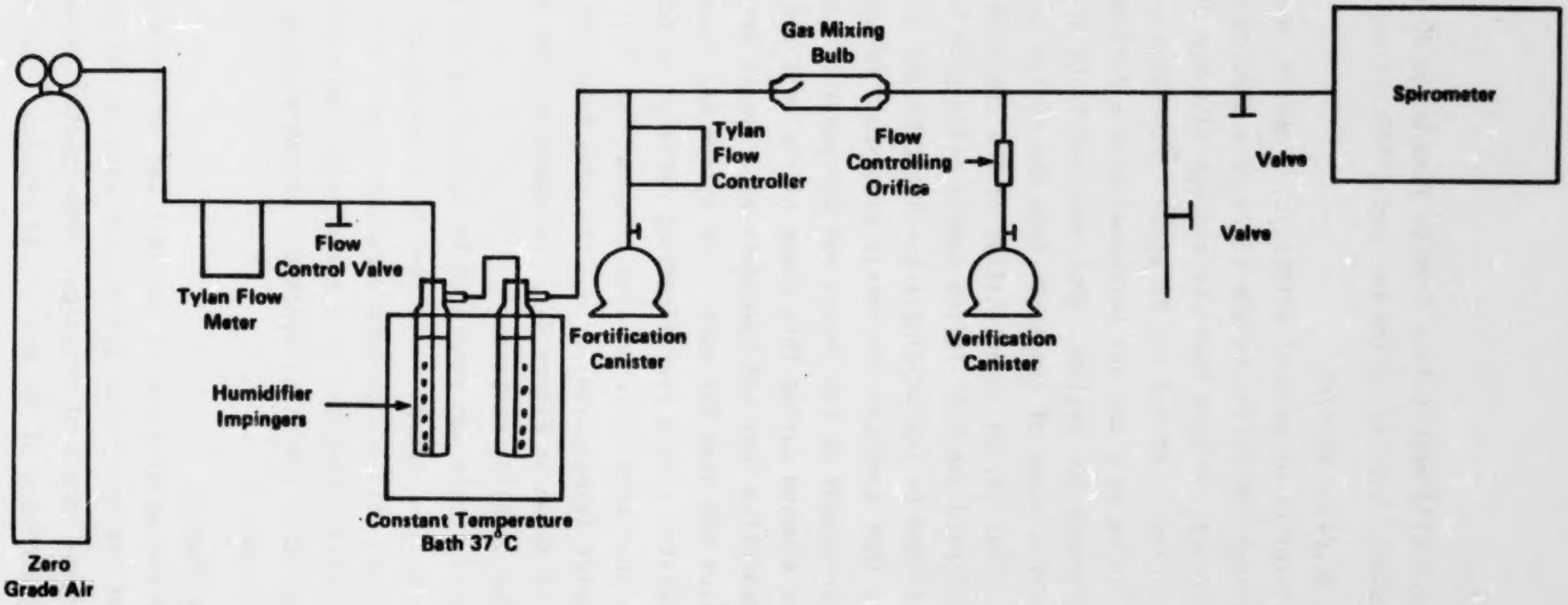
Zero
Grade Air
Tylan Flow
Meter
Flow
Control Valve
Humidifier
Impingers
Constant Temperature
Bath 37°C
Fortification
Canister
Tylan
Flow
Controller
Gas Mixing
Bulb
Flow
Controlling
Orifice
Verification
Canister
Valve
Valve
Spirometer

Figure B-2. Synthetic breath generator including verification canister and switching valves prior to spirometer. The air contains 4.8% CO_2.

TABLE B-3. TARGET COMPOUNDS FOR ADSORPTIVE LOSS AND CARRYOVER EXPERIMENTS

Compound	Conc - Low Level, µg/m³	Conc - High Level,[a] µg/m³
Vinylidene chloride	5.0	49
Methylene chloride	5.4	54
trans-1,2-Dichloroethylene	5.2	51
1,1-Dichloroethane	5.6	56
cis-Dichloroethylene	5.3	52
Chloroform	5.1	51
1,1,1-Trichloroethane	5.5	55
Carbon tetrachloride	5.5	54
Benzene	5.4	54
Trichloroethylene	5.0	50
Toluene	5.3	50
n-Octane	4.8	48
Tetrachloroethylene	5.6	55
1,2-Dibromoethane	6.0	59
Chlorobenzene	5.3	53
Ethylbenzene	5.3	53
p-Xylene	5.3	53
o-Xylene	5.4	53
Styrene	5.6	56
1,1,2,2-Tetrachloroethane	5.4	54
n-Decane	5.0	50
m-Dichlorobenzene	5.3	52
p-Dichlorobenzene	5.4	53
o-Dichlorobenzene	5.4	53
n-Dodecane	5.1	51
4-Phenylcyclohexene	5.4	54

[a] Used only in carryover experiments.

breath samples each with low levels of organics (5 $\mu g/m^3$). If, upon analysis, the first breath sample was found to have lower levels than the second, then the losses were probably due to adsorption. To assure that variations in the synthetic breath generator did not provide erroneous results, a verification canister was used to simultaneously collect an upstream sample simultaneously for comparison to the sampling canister that is part of the spirometer. In this manner, a % recovery for the first and second breath samples was calculated.

A flow rate of 6.2 standard L per minute (Slpm) of air with CO_2 and humidity was mixed with the analytes to provide the low concentration levels shown in Table 4-3. The mixture was passed through the valve shunting it away from the spirometer prior to beginning the experiment. In this manner, the synthetic stream could be established without "conditioning" the surfaces of the spirometer. After equilibration of the stream, a clock was started and the two valves, immediately before the spirometer in Figure 4-2, were reversed so that the mixture flowed into the spirometer. Four seconds later the valves were reversed to shunt (vent) the flow, then four seconds later flow was switched back to the spirometer. This switching was designed to simulate an actual breathing pattern (approximately eight breaths per minute) in order to properly fill the exhaust tube of the spirometer. This breathing cycle was carried out four times then on the fifth "exhale" the sampling with the verification and sampling canisters was started simultaneously. Each canister had a 2.3 L/min orifice (rated at full vacuum) so that sampling for 2.0 min would collect approximately 4.6 L in a 6 L canister. When sampling by the canisters was complete, the flow was left shunted away from the spirometer.

The experiments were carried out as indicated in Table B-4, where each replicate collection was started with a cleaned and dried spirometer. Within each replicate set, the spirometer was reused approximately 5 min later for the second sample collection. During this time, the canisters were replaced and the air stream was vented before the spirometer. The zero concentration air was used to check for organic background contamination in the synthetic breath generator when the fortification canister was detached.

The spirometer was recycled (cleaned and dried) by rinsing the mouthbit and valves with Milli-Q™ treated water then baking the parts in a vacuum

TABLE B-4. SAMPLE COLLECTION REGIMEN FOR THE ADSORPTIVE LOSS EXPERIMENTS

Replicate No.	Experimental Description
1	Zero conc. level[a] Low conc. level Low conc. level
2	Low conc. level Low conc. level
3	Low conc. level Low conc. level

[a] To determine VOC background in the synthetic breath generator and spirometer.

oven at 105°C for at least 30 min. The exhaust tube was simply backflushed with helium until condensation on the walls was removed. Once the apparatus was cooled and reassembled, it was ready to be reused.

The analysis of the collected air samples were carried out using the same procedure as for the filtering experiments, except that a somewhat different set of ions were monitored during GC/MS analysis.

Carryover Studies

Another area of interest was how well the spirometer would perform for the collection breath sample with a high concentration of organics immediately followed by a breath sample with a low VOC concentration. Any carryover would make the characterization of rapidly-changing breath levels difficult. This experiment was carried out by generating and collecting a high concentration (50 $\mu g/m^3$) breath sample through the spirometer followed by shunting the flow away while the level was adjusted to a low concentration (5 $\mu g/m^3$). After equilibration (10 min), the low concentration sample was collected in the same manner as for the high concentration sample. The "breathing" cycle was held constant at 8 sec as before and the other parameters were unchanged. The spirometer was cleaned, as described above, between each replicate sample collection. The sample collection regimen used is shown in Table B-5.

The analyses were carried out using the GC/MS system and the same method as for the adsorptive loss experiments.

PORTABLE SPIROMETER DESIGN

A design for a portable spirometer for collecting VOCs in alveolar breath over a concentration range from low ppb to ppm was formulated based on the results of previously described experiments. The primary design goals were portability and ease of use for both the operator and participant. The design was driven by the desire to collect a representative sample of alveolar breath in stainless steel canisters in under two minutes. Breath samples could then be stored for later analysis by GC/MS. Based on design goals, a number of desirable features were incorporated into the final design and are briefly described here.

Portability

The need for a portable device drove the entire design process. Our previous spirometer design required a large van for transport and required

TABLE B-5. SAMPLE COLLECTION REGIMEN FOR THE CARRYOVER EXPERIMENTS

Replicate No.	Experimental Description
1	High conc. level Low conc. level
2	High conc. level Low conc. level
3	High conc. level Low conc. level Zero conc. level[a]

[a] To determine background levels from carryover.

the participant going to the van to supply the breath sample. The goal for this alveolar spirometer was to produce a device that could be easily carried by one person. Such a portable device could be carried to the participant in their home or workplace, and could be easily transported to the sampling site.

Speed of Sample Collection

The whole breath spirometer used in previous studies required approximately 10 minutes for set-up and another 15 to 20 minutes for sample collection. This length of time was inconvenient during field studies of human exposures and created difficulties in time resolution during kinetic studies on chemical elimination from the body. The design goal for the alveolar spirometer was a device that could be set-up in under 5 minutes and could collect breath samples in 2 minutes or less. Such a device should ease the time burden during field studies and improve the accuracy of measuring the initial decay rate during elimination kinetics studies.

Ease of Use

Part of the improvement in sample collection times will result from making the alveolar device simple for the operator and participant to use. For ease of use and portability reasons, no pumps, bags, gas cylinders, or electronic components were incorporated into the spirometer design. The operator is required only to connect tubing and canisters in the system and then open and close the canister valves at specified times. Sample collection is driven by the pressure difference between the evacuated canister and the breath collection tube. The sampling rate is governed by a simple fixed needle orifice. Breath samples are contained in a simple long open Teflon tube. Clean inhale air, requiring no humidification, is provided when the participant inhales through respirator cartridges charcoal filled. The flow of breath is directed using custom designed unidirectional Teflon float ball valves.

Participant convenience is improved since the breath sample is provided in under 2 minutes instead of the 4 to 6 minutes required using the previously designed, whole breath spirometer. A new Teflon mouthbit was designed to increase participant comfort and new, foam padded noseclips have been obtained to ease the discomfort encountered when the participant seals his nasal airway.

The spirometer was also designed so that it could be used easily by people of all ages. A mounting plate was designed to pivot up on hinges and then slide partially out of the case. This design will allow placement of the device on a table with a height adjustment so people of different sizes can comfortably reach the mouthbit.

Duplicate Sample Collection

In order to measure precision of the sampling and analysis procedure, the spirometer must be capable of duplicate sample collection. This feature was incorporated into the spirometer design so that simultaneous sampling of a breath sample into two canisters can be performed.

Prevention of Pathogen Transfer

Any spirometer system used for multiple participants must prevent the potential spread of pathogens from one participant to the next. The spirometer must also be designed for disinfection under field use where elaborate equipment is not available. With this in mind, all spirometer parts were selected so that the materials could be autoclaved or disposed of and that the parts could be easily disassembled for cleaning.

Tenax Sampling Option

The alveolar spirometer was designed with the idea that it may be desirable in the future to collect breath samples on Tenax cartridges instead of canisters. This capability would expand the range of target compounds available to this method. The design incorporated a removable mounting plate so that a new plate can be installed that will hold a pump and Tenax cartridges should this be required in future work.

SECTION 5
RESULTS AND DISCUSSION

SOURCES OF AIR FOR INHALATION

Background from Filter

The quantifiable limits (QLs) for the compounds studied in these experiments are listed in Table B-6 for various breath volumes analyzed. In the following tables, the QLs are shown for the analytical volumes used in that experiment. The analytical results for the air samples collected to determine the background from the VOC are shown in Table B-7. In general, the background was quite low. Only dichloromethane and tetrachloroethylene were measured at levels above the QL. Concurrent measurements of the laboratory air indicated relatively high levels of the chlorinated compounds. It is possible that chlorinated compounds detected in the samples might well be derived from residual lab air in the system after filter or cannister installation. Consequently, the true source of these compounds is unclear. The presence of organic compounds, even at these levels, could present a problem for the analysis of compounds in breath if the exposure level was very low. It should be noted that the filtration flow rate used here was 2 L/min. In an application where air is inhaled through the filters, the flow rate will be much faster, approximately 20 L/min. Thus, the low flow rate used for this background check maximizes the likelyhood of detecting compounds released from the filter cartridge and represents a worst case situation. The final spirometer design will allow for the collection of spirometer blanks for evaluating contamination during field studies.

Breakthrough Volumes of Target Compounds

The results of the experiments designed to challenge the cartridge with low levels of organic compounds using a continuous air flow are shown in Table B-8. Overall, the data indicate that the charcoal filters perform very well. Dichloromethane was the only compound consistently detected and it was measured at levels near the QL of the method and less than 0.4% of the inlet concentration.

TABLE B-6. ESTIMATED QUANTIFIABLE LIMITS FOR TARGET COMPOUNDS FOR CANISTER AIR ANALYSES USING MID

Compound	Conc. ($\mu g/m^3$) for Volume Analyzed		
	20 mL	150 mL	200 mL
Isopentane	12	1.7	1.2
n-Pentane	15	2.0	1.5
2-Methylhexane[a]	3.5	0.5	0.35
3-Methylhexane[a]	3.5	0.5	0.35
Vinylidene chloride	6.5	0.9	0.65
1,1,1-Trichloroethane	33	4.4	3.3
Tetrachloroethylene	18	2.4	1.8
2-Methylpentane	16	2.1	1.6
Benzene	12	1.6	1.2
Carbon tetrachloride	5.0	0.7	0.5
Chloroform	5.0	0.7	0.5
Dichloromethane	17	2.3	1.7
Toluene	4.0	0.5	0.4
p-Xylene	2.0	0.3	0.2
n-Nonane	3.5	0.5	0.35
n-Decane	5.0	0.7	0.5
n-Undecane[a]	5.0	0.7	0.5
n-Butanol[b]	40	40	40
n-Butyl acetate	40	40	40

[a] Concentrations are estimates based on similar compounds.

[b] Minimum ion intensity detectable.

TABLE B-6. ESTIMATED QUANTIFIABLE LIMITS FOR TARGET COMPOUNDS FOR CANISTER AIR ANALYSES USING MID

Compound	Conc. ($\mu g/m^3$) for Volume Analyzed 20 mL	150 mL	200 mL
Isopentane	12	1.7	1.2
n-Pentane	15	2.0	1.5
2-Methylhexane[a]	3.5	0.5	0.35
3-Methylhexane[a]	3.5	0.5	0.35
Vinylidene chloride	6.5	0.9	0.65
1,1,1-Trichloroethane	33	4.4	3.3
Tetrachloroethylene	18	2.4	1.8
2-Methylpentane	16	2.1	1.6
Benzene	12	1.6	1.2
Carbon tetrachloride	5.0	0.7	0.5
Chloroform	5.0	0.7	0.5
Dichloromethane	17	2.3	1.7
Toluene	4.0	0.5	0.4
p-Xylene	2.0	0.3	0.2
n-Nonane	3.5	0.5	0.35
n-Decane	5.0	0.7	0.5
n-Undecane[a]	5.0	0.7	0.5
n-Butanol[b]	40	40	40
n-Butyl acetate	40	40	40

[a] Concentrations are estimates based on similar compounds.

[b] Minimum ion intensity detectable.

TABLE B-7. CONCENTRATIONS (ug/m^3) OF TARGET COMPOUNDS FOUND IN FILTERED LABORATORY AIR[a]

	First Cartridge[b]		Second Cartridge			Third Cartridge		
Compound	35 min	unfiltered	0 min	35 min	unfiltered	0 min	35 min	unfiltered
Vol. Analyzed:	150 mL	150 mL	200 mL	200 mL	150 mL	200 mL	200 mL	200 mL
Dichloromethane	4.2	35	2.9	3.2	D[c]	T[d]	T	13.4
Chloroform	ND[c]	67	ND	ND	D	T	ND	33
1,1,1-Trichloroethane	ND	513	ND	ND	D	T	T	16.6
Benzene	T	3.9	T	T	D	T	T	2.3
Toluene	ND	10.5	ND	ND	D	T	ND	10.1
Tetrachloroethylene	ND	12.7	ND	ND	ND	8.6	5.2	7.7
_n_-Nonane	ND	0.5	ND	ND	ND	T	ND	ND
_n_-Decane	ND	0.83	ND	ND	ND	T	ND	T

[a] Samples of filtered air were collected starting at 0 or 35 min. Unfiltered air samples were collected immediately before or after the corresponding set of filtered air samples were collected.

[b] The 0 min sample was not analyzed by MID.

[c] D = Detected by full scan but not quantitated; ND = not detected.

[d] T = Trace level detected, below QL.

TABLE B-8. CONCENTRATIONS OF TARGET COMPOUNDS IN AIR WITH CONTINUOUS FILTERING AT LOW CONCENTRATIONS

Compound	QL (ug/m^3)	Conc. in Unfiltered air (ug/m^3) 0 L	2022 L	Conc. in Filtered Air (ug/m^3) 0 L	82 L	490 L	987 L	2022 L
	Volume Analyzed:	20 mL	10 mL	200 mL	200 mL	200 mL	200 mL	200 mL
Isopentane	1.25	>1720	795	ND[a]	ND	ND	ND	ND
1-Pentane	1.5	1860	990	ND	ND	ND	ND	ND
2-Methylhexane[b]	0.35	1.8	ND	ND	ND	ND	ND	ND
3-Methylhexane[b]	0.35	4.2	4.7	T[c]	T	T	0.49	T
Vinylidene chloride	0.65	>1090	855	ND	ND	ND	ND	ND
1,1,1-Trichloroethane	3.3	2140	1860	T	T	T	T	T
2-Methylpentane	1.6	900	1290	ND	ND	ND	ND	ND
Benzene	1.2	780	773	T	T	T	T	T
Carbon tetrachloride	0.5	3310	2820	ND	ND	ND	ND	ND
Chloroform	0.5	710	6190	T	ND	ND	ND	ND
Dichloromethane	1.7	710	552	2.5	2.0	T	1.7	2.6
Toluene[b]	0.4	2.8	2.2	ND	ND	ND	ND	ND
p-Xylene[b]	0.2	1.3	ND	ND	ND	ND	ND	ND
n-Butanol	NA[d]	NT[e]	35300[f]	NT	NT	NT	NT	ND
n-Butyl acetate	0.4	NT	14200[f]	NT	NT	NT	NT	72[f]

[a] ND means no ion detected.

[b] Not added to mixture.

[c] T = trace: detected but below QL.

[d] NA = not determined.

[e] NT = not tested.

[f] Ion intensity for 100 mL.

Analogous results for the experiment using higher level of organics are shown in Table B-9. In this case, the dichloromethane levels found in the samples collected at 0 and 320 L represent less than 0.2% of the inlet levels. That such levels were not measured in the blanks and were measured in the filtered air samples suggests that the flow rate might be too rapid for complete removal of the dichloromethane. To overcome this, we have designed the spirometer system to operate with two cartridges in parallel such that the flow rate through each cartridge is reduced by 50%. As noted in the background experiments, the presence of this compound could be an artifact of the laboratory environment where dichloromethane is commonly used. This aspect does indicate caution when planning and interpreting measurements of dichloromethane at low levels. The data also show that at 646 L, dichloromethane has begun to break through the sorbent bed. Therefore, a volume up to 320 L per cartridge would provide clean air for inhalation for conditions similar to these experiments.

Effect of Filter Storage and Reuse

The results of the experiment where the cartridge was used intermittently over 5 days and stored between uses are shown in Table B-10. These data are consistent with those of Table B-9 in that increased levels of dichloromethane were measured in the sample collection begun at 643 L (day 2) suggesting a safe volume of 320 L. Thus, under these conditions, the effect of storage and multiple use of the filter is minimal.

CHOICE OF OPTIMAL CANISTER SIZE

As indicated in the experimental section, we wished to choose a canister as small as possible for use in the portable spirometer system. A 1 L Summa polished canister was evaluated according to the criteria outlined above. The results of these repeated analyses are shown in Table B-11. The data show that the vacuum and flow rate were acceptable for the first two analyses. With the third analysis, the flow rate dropped below 20 sccm and the canister vacuum increased to 16"Hg which would result in difficuties with quantitation. Consequently, we decided that a larger canister was needed. According to Scientific Instrumentation Specialists, the supplier of the canisters, the next larger canister that could be manufactured from readily available materials would result in a volume of 1.8 L. Given that two good samples could be withdrawn from the 1 L

TABLE B-9. CONCENTRATIONS OF TARGET COMPOUNDS IN AIR WITH APPROXIMATELY CONTINUOUS FILTERING AT HIGHER CONCENTRATIONS

		Conc. in air (mg/m^3)		Conc. in Air (ug/m^3)				
Compound	QL (ug/m^3)	650 L	940 L	0 L	320 L	650 L	960 L	1290 L
Volume Analyzed:		20 mL	20 mL	200 mL	200 mL	200 mL	200 mL	200 mL
Isopentane	1.2	5.4	0.49	ND[a]	ND	ND	ND	ND
n-Pentane	1.5	7.0	1.50	T[b]	T	T	T	T
Vinylidene chloride	0.65	6.0	2.4	ND	ND	ND	ND	ND
1,1,1-Trichloroethane	3.3	16	13	ND	ND	ND	ND	ND
2-Methylpentane	1.6	13	6.4	ND	ND	ND	ND	ND
Benzene	1.2	>6.8	>7.0	T	T	T	T	T
Carbon tetrachloride	0.5	26	23	ND	ND	ND	ND	ND
Chloroform	0.5	6.7	6.1	T	0.66	T	T	T
Dichloromethane	1.7	5.3	3.6	7.2	9.0	24	96.	330.
n-Decane[c]	0.50	ND	ND	ND	ND	ND	T	ND
n-Butanol	NA[d]	NT[e]	33265[f]	NT	NT	NT	NT	128[d]
n-Butyl acetate	0.4	NT	178930[f]	NT	NT	NT	NT	147[d]

[a] ND means not detected.

[b] T = trace; detectecd but below QL.

[c] Not added to mixture.

[d] NA = not determined.

[e] NT = not tested.

[f] Ion intensity normalized to 100 mL; 55.6 mL analyzed.

TABLE B-10. CONCENTRATIONS OF TARGET COMPOUNDS IN AIR COLLECTED OVER 5 CYCLES (DAYS)

	Conc. in air (mg/m^3)		Conc. in air (ug/m^3)				
Compound	Day 4: Start	Day 4: End	Day 0	Day 1	Day 2	Day 3	Day 4
Volume Analyzed:	20 mL	20 mL	200 mL	200 mL	200 mL	200 mL	200 mL
Isopentane	7.1	1.3	ND[a]	ND	ND	ND	ND
n-Pentane	8.2	2.3	ND	ND	T[b]	ND	ND
2-Methylhexane[c]	ND	ND	ND	ND	ND	ND	ND
3-Methylhexane[c]	ND	ND	ND	ND	ND	ND	ND
Vinylidene chloride	7.5	4.1	ND	ND	ND	ND	T
1.1.1-Trichloroethane	18	18	ND	ND	ND	T	T
2-Methylpentane	12	7.8	ND	ND	ND	ND	T
Benzene	7.8	8.0	T	T	T	T	T
Carbon tetrachloride	28	30	ND	ND	ND	ND	ND
Chloroform	6.1	6.6	ND	ND	ND	ND	ND
Methylene chloride	5.1	4.1	2.8	4.2	61	190	370
n-Undecane[c]	ND	ND	ND	ND	ND	T	ND
n-Butanol	NT[d]	20,200[e]	NT	NT	NT	NT	ND
n-Butyl acetate	NT	107,400[e]	NT	NT	NT	NT	140[e,f]
Cumulative Volume at start of sample collection			0	323	643	966	1287

[a] ND = ion not detected.

[b] T = trace detected (below quantifiable limit).

[c] Not added to mixture.

[d] NT = not tested.

[e] Ion intensity for 100 mL.

[f] 147.7 mL analyzed.

TABLE B-11. RESULTS OF MULTIPLE ANALYSIS CAPACITY OF 1-LITER CANISTERS

Analysis Number	Canister Vacuum ("Hg)	Trapping Flow[a] (sccm)
1	3.8 (initial) 7.3 (final)	20 throughout
2	11.8 (final)	20 initial and until 2 minutes 19.8 final
3	16 (final)	20 initial 18.6 after 2 minutes 16.5 after 3 minutes (final)

[a] Total trapping time is 10 minutes.

samples, and probably four or five, could be withdrawn from a 1.8 L canister. This larger canister is approximately 5 inches in diameter and 10 inches tall compared to 4" by 9" for the 1 L canister. This small increase in size was not anticipated to cause any major problem with portability so the 1.8 L canister was chosen for use in the final system.

ADDITIONAL RECOVERY STUDIES

Adsorption Studies

The results of the experiment to study the adsorptive behavior of the spirometer to the test compounds are shown in Table B-12 . The first and second uses of the spirometer are grouped together and the replicate number is indicated. The mean recovery, relative to the verification canister, of the first use was 94% and was 100% for the second use. This shows that there are no major losses associated with adsorption. At the low levels used in this experiment, the lesser volatile compounds n-dodecane and 4-phenylcyclohexene were poorly recovered. Thus, compounds more volatile than these two compounds can most likely be collected successfully with the new spirometer. Where the most accurate measurements possible are required, a small amount of conditioning of the spirometer might be necessary to maximize the recoveries of the organic compounds. This could be accomplished by requiring the study participant to breath through the device for two minutes prior to the collection of the sample. When the spirometer is to be used multiple times by the same person, as for kinetic studies, this conditioning would only be needed for the first sample.

Carryover Studies

The results of the carryover experiments are shown in Table B-13. The high level and the low level results for each high level/low level pair are grouped together. If carryover were a problem, recoveries greatly in excess of 100% would be expected for the low level samples. This clearly was not the case indicating that, in general, there are no problems associated with the carryover of the test compounds. Note however, that the percent recoveries for n-dodecane and 4-phenylcyclohexene in the low level cases in this experiment are higher than those in the adsorptive loss experiment. This suggests that as analytes become less volatile, they are

TABLE B-12. PERCENT RECOVERY[a] FROM ADSORPTIVE LOSS EXPERIMENTS FOR THE FIRST AND SECOND SPIROMETER USE FOR EACH SAMPLING PAIR

		First Use						Second Use					
		% Recovery						% Recovery					
Compound	*m*/*z*[b]	1	2	3	Mean	SD	%RSD	1	2	3	Mean	SD	%RSD
Vinylidene chloride	61	93	98	97	96	2	2	97	95	92	95	2	2
Dichloromethane	84	99	90	100	96	4	5	78	93	87	86	6	7
trans-Dichloroethylene	61	95	103	98	99	3	3	99	97	104	100	3	3
1.1-Dichloroethane	63	94	98	92	95	3	3	91	103	99	98	5	5
cis-Dichloroethylene	61	92	91	87	90	2	2	92	105	96	98	5	6
Chloroform	83	102	125	110	112	10	8	86	106	119	104	13	13
1.1.1-Trichloroethane	61	99	96	86	94	5	6	92	103	100	98	5	5
Carbon tetrachloride	82	128	72	117	106	24	23	120	114	107	114	5	5
Benzene	78	102	94	90	96	5	5	105	90	96	97	6	6
Trichloroethylene	60	92	97	95	95	2	2	104	95	100	100	4	4
Toluene	91	90	96	95	94	3	3	99	100	100	100	0	0
n-Octane	57	91	90	93	91	1	1	104	95	96	98	4	4
Tetrachloroethylene	59	84	98	80	87	8	9	95	87	71	84	10	12
1.2-Dibromoethane	107	100	94	96	97	2	2	104	100	94	99	4	4
Chlorobenzene	77	101	89	93	94	5	5	97	93	94	95	2	2
Ethylbenzene	91	97	97	94	96	2	2	102	100	102	101	1	1
p-Xylene	91	96	96	89	94	3	4	99	102	99	100	1	1
o-Xylene	91	94	98	90	94	3	4	100	99	97	99	1	1
Styrene	104	92	96	79	89	7	8	110	108	105	108	2	2
1.1.2.2-Tetrachloroethane	83	100	92	92	95	4	4	105	100	92	99	5	5
n-Decane	57	93	93	98	95	2	3	107	106	102	105	2	2
m-Dichlorobenzene	75	85	95	89	90	4	5	91	100	96	96	4	4
p-Dichlorobenzene	75	102	92	97	97	4	4	105	108	107	106	1	1
o-Dichlorobenzene	75	110	94	97	100	7	7	102	95	108	102	5	5
n-Dodecane	57	62	61	70	64	4	4	106	129	130	121	11	9
4-Phenylcyhclohexene	104	ND[c]	ND	54	54	--	--	ND	114	92	103	11	10
AVERAGE		96	94	91	94	2	2	100	101	99	100	1	1

[a] Percent recovery relative to the verification canister before the spirometer.

[b] Ion monitored during sample analysis.

[c] ND = not detected.

TABLE B-13. PERCENT RECOVERY[a] RELATIVE TO VERIFICATION SAMPLE FOR EACH HIGH LEVEL/LOW LEVEL PAIR TO TEST CARRYOVER

		High Level						Low Level					
		% Recovery						% Recovery					
Compound	*m*/*z*[b]	1	2	3	Mean	SD	%RSD	1	2	3	Mean	SD	%RSD
Vinylidene chloride	61	79	102	101	94	11	11	95	97	90	94	3	3
Dichloromethane	84	93	104	103	100	5	5	100	93	105	99	5	5
trans-Dichloroethylene	61	81	95	107	95	10	11	98	94	87	93	5	5
1,1-Dichloroethane	63	80	99	98	92	9	10	99	89	88	92	5	6
cis-Dichloroethylene	61	104	105	103	104	1	1	104	92	92	96	5	6
Chloroform	83	119	97	100	105	9	9	101	104	102	102	1	1
1,1,1-Trichloroethane	61	103	102	101	102	1	1	105	89	93	96	7	7
Carbon tetrachloride	82	111	98	101	103	6	6	107	84	95	95	10	10
Benzene	78	116	98	102	105	8	7	98	103	94	99	4	4
Trichloroethylene	60	100	101	100	100	1	1	107	103	85	99	9	10
Toluene	91	124	100	59	94	27	28	99	87	93	93	5	6
n-Octane	57	89	97	91	92	3	4	92	90	87	90	2	2
Tetrachloroethylene	59	94	102	106	101	5	5	101	84	106	97	10	10
1,2-Dibromoethane	107	122	100	101	107	10	10	88	86	105	93	8	9
Chlorobenzene	77	106	101	99	102	3	3	98	83	91	91	6	7
Ethylbenzene	91	114	103	99	105	6	6	95	82	94	91	6	7
p-Xylene	91	119	99	97	105	10	10	99	81	90	90	7	8
o-Xylene	91	110	104	104	106	3	4	94	86	90	90	3	4
Styrene	104	126	103	98	109	12	11	105	75	87	89	12	14
1,1,2,2-Tetrachloroethane	83	113	106	105	108	3	3	100	101	90	97	5	5
n-Decane	57	98	100	94	97	2	2	100	81	97	92	8	9
m-Dichlorobenzene	75	107	98	107	104	4	4	94	88	99	93	5	5
p-Dichlorobenzene	75	109	104	104	105	3	3	109	92	96	99	7	7
o-Dichlorobenzene	75	105	98	97	100	4	4	111	79	99	96	13	14
n-Dodecane	57	64	92	98	85	15	17	76	60	110	82	21	26
4-Phenylcyhclohexene	104	ND[c]	92	90	91	43	47	151	46	93	97	43	44
AVERAGE		103	100	99	101	2	2	99	86	94	93	5	6

[a] Percent recovery relative to the verification canister before the spirometer.

[b] Ion monitored during sample analysis.

[c] ND = not detected.

not released easily from the spirometer. The results for these two compounds in both experiments are consistent and suggest a volatility limit for compounds to be sampled with this device.

PORTABLE SPIROMETER CONSTRUCTION

Six portable spirometers were constructed for the collection of VOCs in alveolar breath. The spirometers were designed to collect breath VOCs at concentrations ranging from low $\mu g/m^3$ (ppb) levels, that might result from environmental exposures, up to mg/m^3 (ppm) levels that might result from occupational exposures. The spirometers were designed and constructed with portability, ease of use, and effective analyte collection as primary goals. Each device can be carried by one person, set-up in the field in less than five minutes, collect alveolar breath samples in less than two minutes. All spirometer materials were chosen to be light weight, to lack analyte adsorption or emission properties, and to allow sterilization or disposal to prevent pathogen transmission between subjects.

A diagram of the portable spirometer is presented in Figure B-3. Detailed part descriptions, corresponding to the numbers on the figure, are presented in Table B-14. The spirometer is housed in an aluminum case to protect the device during shipment and to provide a rugged support frame for the interior components. All components are attached to an aluminum plate that in turn is mounted on pivoting slides. These slides allow the entire mounting plate to slide out horizontally and elevate vertically from pivot points at the rear of the case. This feature is incorporated so that the spirometer mouthbit can be easily reached by children and adults when the spirometer is placed on a table. A simple lever is used to adjust the mounting plate to six different heights to accommodate a wide range of participant heights. The overall device size is 61.5 x 48 x 22.5 cm when the case is closed. The device weighs 10.5 kg with two 1.8 L canisters enclosed. Spare parts can be carried in the space beneath the mounting plate.

Spirometer functions were designed to be as simple as possible, with no electricity, air cylinders, humidifiers, or collection bags required for operation. A brief description will be provided here on the intended

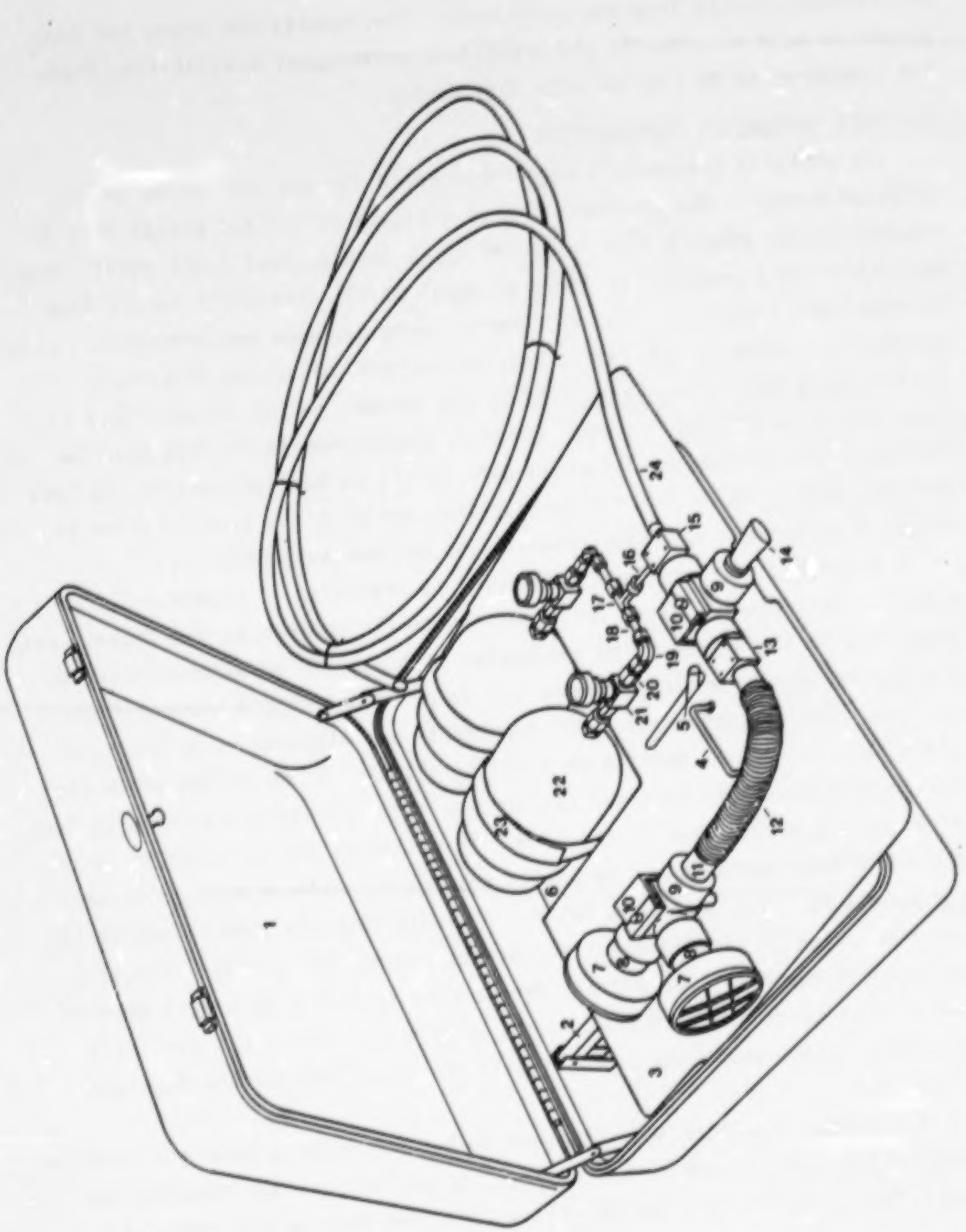
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Figure B-3 Portable spirometer for the collection of VOCs in alveolar breath.

TABLE B-14. PORTABLE SPIROMETER PARTS LIST[a]

1. Carrying case
Source: Jensen Tools Inc., Phoenix, AZ
Dimensions: Interior dimensions 60 x 44 x 22 cm
Material: Aluminum with rubber gasket

2. Mounting plate slide
Source: Local hardware store, custom construction at RTI
Dimensions: 40 cm long, 1.3 cm wide
Material: Aluminum channel

3. Mounting plate
Source: Comfort Engineers, Durham, NC
Dimensions: Overall 58 x 43 x 0.32 cm
Material: Aluminum

4. Handle
Source: Local hardware store
Dimensions: 11 x 3.2 cm
Material: Aluminum

5. Vertical elevation lever
Source: Edgecomb Steel, Charlotte, NC
Dimensions: 24 cm long, 1.2 cm diameter rod
Material: Aluminum

6. Canister well plate
Source: Comfort Engineers, Durham, NC
Dimensions: 30.6 x 19.5 x 0.32 cm
Material: Aluminum

7. Inhale respirator cartridge
Source: Survivair®, Santa Ana, CA
Dimensions: 8.8 cm diameter, 3.5 cm deep
Materials: Activated charcoal encased in plastic with gauze supports

8. Respirator cartridge adapter
Source: Custom construction at RTI, O-ring from Dixie Bearings, Durham, NC
Dimensions: One end threaded to mate cartridge, other end 2.54 cm o.d., 1.3 cm i.d.
Materials: Adapter is Teflon® TFE, O-ring is Viton®

9. Union-T
Source: Filtration Technology, Inc., Greensboro, NC
Dimensions: 2.54 cm i.d.
Material: Teflon® TFE

(continued)

TABLE B-14 (cont'd.)

10. Union clamp
    - Source: Local hardware store, custom constructed
    - Dimensions: 6.0 x 4.4 x 4.2 cm
    - Materials: Aluminum angle, aluminum channel, steel thumbscrew, steel spring

11. Tubing adapter
    - Source: Custom construction at RTI
    - Dimensions: 2.54 cm o.d. on union-T end, tapers 2.1 to 1.9 cm o.d. on tubing end, 1.2 cm i.d.
    - Material: Teflon® TFE

12. Flexible polyethylene tubing
    - Source: Dayco Corp., Dayton, OH
    - Dimensions: 1.9 cm i.d., 2.5 cm o.d., 18 cm long
    - Material: Polyethylene, flexible

13. Unidirectional inhale valve
    - Source: Custom constructed at RTI
    - Dimensions:
      - (a) Inlet end tapers 2.1 to 1.9 cm o.d., 12 cm i.d.
      - (b) Union-t end 2.54 cm o.d., 12 cm i.d.
      - (c) Float ball 1.0 cm diameter
      - (d) Valve interior orifices 0.6 cm i.d.
    - Materials: Body and ball are Teflon® TFE, screws are stainless steel

14. Mouthbit
    - Source: Custom constructed at RTI
    - Dimensions: Overall length 7.5 cm, Union end 2.54 cm o.d. and 1.2 cm i.d., mouth end 2.8 cm wide x 1.4 cm deep
    - Material: Teflon® TFE

15. Unidirectional exhale valve
    - Source: Custom constructed at RTI
    - Dimensions:
      - (a) Union-t end 2.54 cm o.d., 12 cm i.d.
      - (b) Outlet end 1.27 cm o.d., 1.2 cm i.d.
      - (c) Float ball 1.0 cm diameter
      - (d) Valve interior orifices 0.6 cm i.d.
    - Materials: Body and ball are Teflon® TFE, screws are stainless steel

16. Sampling port
    - Source: Custom constructed at RTI
    - Dimensions: 5.1 cm long, 0.6 cm o.d., 0.4 cm i.d.
    - Material: Stainless steel

(continued)

TABLE B-14 (cont'd.)

17.	Union-T	
	Source:	Swagelok®, Raleigh Valve and Fitting, Raleigh, NC
	Dimension:	0.6 cm tube o.d. fitting
	Material:	Stainless steel except Teflon® TFE ferrules at sampling port connection
18.	Connector tubing	
	Sources:	(a) Swagelok® fittings, Raleigh Valve and Fitting, Raleigh, NC (b) Tubing, Atlantic Plastics, Raleigh, NC
	Dimensions:	4.4 cm long, 0.6 cm o.d., 0.4 cm i.d.
	Materials:	(a) Fittings are stainless steel (b) Tubing is Teflon® TFE
19.	Elbow union	
	Source:	Swagelok®, Raleigh Valve and Fitting, Raleigh, NC
	Dimensions:	0.6 cm tube o.d. fitting
	Materials:	Stainless steel
20.	Flow control orifice	
	Source:	(a) Orifice needle Becton Dickinson, Rutherford, NJ (b) Fittings, Swagelok®, Raleigh Valve and Fitting, Raleigh, NC (c) Septum, Supleco, Bellefonte, PA
	Dimensions:	(a) Needle, 22 gauge, 2.2 cm long (b) Tube, 2.4 cm long, 0.6 cm o.d., 0.4 cm i.d. (c) Septum, 0.75 cm long, 0.6 cm diameter
	Materials:	(a) Needle and fittings are stainless steel (b) Septum is Thermogreen® rubber
21.	Canister valve	
	Source:	Nupro Co., Willoughby, OH
	Dimensions:	0.6 mm tube fittings on bellows valve
	Materials:	Stainless steel
22.	Canister	
	Source:	Scientific Instrumentation Specialist, Moscow, ID
	Dimensions:	Nominal 1.8 L cylindrical, 25 cm long, 12.7 cm diameter
	Materials:	Summa® polished stainless steel
23.	Canister straps	
	Source:	Locally purchased
	Dimensions:	50 cm long, 2 cm wide
	Material:	Nylon straps with Velcro® closure

(continued)

TABLE B-14 (cont'd.)

24. Breath containment tube
    Source: Atlantic Plastics, Raleigh, NC
    Dimensions: 1.27 cm i.d., 0.076 cm wall thickness, 762 cm long
    Material: Teflon® FEP

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[a] Part number corresponds to numbers in Figure B-3.

sample collection procedure with a discussion of the function of each component. Initial set-up is accomplished by placing the spirometer components in their proper places. A 1.8 L stainless steel canister is placed into the holding well and strapped into place (two canisters are used if duplicate samples are to be collected). A previously sterilized mouthpiece unit, consisting of an inhale valve, exhale valve, mouthbit, and sampling orifice, are clamped into place. The Teflon and stainless steel valves are custom built with a Teflon float ball to provide uni-directional flow (Figure B-4). These valves will operate over the angles created by pivoting the mounting plate and can be autoclaved for sterilization. The orifice union is connected to the canister valve. A precleaned polyethylene tube is connected, using a friction fit, from the respirator outlet to the inhale valve inlet. The Teflon breath containment tube is connected, using a friction fit, to the exhale valve outlet. The participant is seated in front of the spirometer and the mounting plate is raised to a height which will be comfortable to the participant. The participant dons pinch-type nose clamps to prevent breathing through the nostrils.

The participant is instructed to place his mouth tightly over the mouthbit and to begin breathing as normally as possible. Some resistance to normal breathing is encountered due to the constrictions of the valves and long breath containment tube. People generally breathe through this device at a slower and deeper rate than is normal which should enhance the portion of alveolar breath being sampled. As the participant inhales, air is pulled through the two charcoal filled respirator cartridges to remove VOCs in the inhale air. The subject is asked to provide four full breaths before sample collection is initiated. This ensures that the spirometer and participant airways are cleared of analytes found in the ambient air at the sampling location. As the participant breathes, clean inhale air passes through the unidirectional inhale valve and into the lungs. As the participant exhales the breath passes out through the unidirectional exhale valve and into the breath containment tube.

Sample collection is initiated at the end of the fourth exhalation by opening the canister valve. The canister is at an initial pressure of 5×10^{-2} torr, so the pressure differential drives the sample collection. Flow control is achieved using a simple fixed needle orifice. The orifice is designed to collect 1.4 L of breath in canisters with a nominal volume of

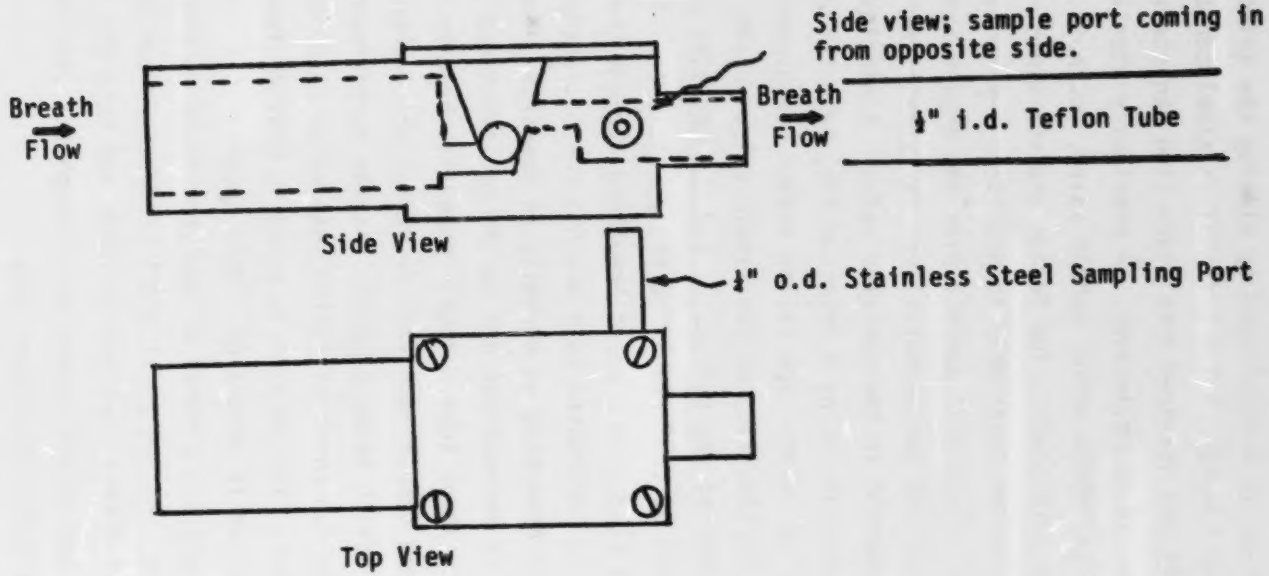
Breath
Flow
Side View
Breath
Flow
Side view; sample port coming in from opposite side.
½" i.d. Teflon Tube
¼" o.d. Stainless Steel Sampling Port
Top View

Figure B-4. Exhale valve and sample port.

1.8 L over a 1.5 min time period. Breath samples in the canisters are maintained at sub-ambient pressures in order to reduce water condensation inside the canisters. Collection of the breath sample is slightly time weighted since the fixed needle is not a critical orifice. The collection rate remains nearly constant from the beginning of the sample collection until the canister reaches approximately 50% of ambient pressure (0.9 L in a 1.8 L canister). From that point, the flow rate decreases approximately 30% until 1.4 L of sample has been collected and the canister valve is closed.

The breath containment tube was designed to allow the collection of breath that is over 95% alveolar by composition. As the participant exhales, the deadspace air from his breathing airways passes rapidly by the sampling part in the exhale valve. The deadspace air is briefly sampled as it passes, but passage time is fast because there is little restriction to its exhalation in the body. The remaining portion of the exhaled breath comes from the alveoli in the lungs, and it is also sampled as it passes by the collection port during exhalation. The volume of alveolar to deadspace air is typically 2:1 to 3:1 and it takes longer to exhale since there is more resistance in the lungs. Therefore, a much larger volume of alveolar air is sampled as compared to deadspace air during each exhalation.

As inhalation begins, a plug of exhaled breath remains in the breath collection tube. The portion of the plug nearest the sampling port represents the last portion of exhaled breath. This last portion is composed entirely of alveolar breath. The breath containment tube dimensions and sample collection rates have been selected so that only alveolar breath is collected from the containment tube while the participant inhales, even if duplicate samples are collected. The participant keeps breathing into the spirometer until sample collection has been completed, then the canister valve is closed and the participant can release his mouth from the mouthbit.

In order to prevent pathogen transmission between participants the entire mouthpiece unit is washed with organic free water and autoclaved between uses. The flexible polyethylene tubing is disposed of after each participant has provided a sample. Breath containment tubes are purged with clean air between uses to remove residual water condensate. As previously described each respirator cartridge is effective in removing ambient air VOCs from air volumes less than or equal to 320 L over several days. We recommend that the cartridges be replaced after the collection of 10 samples or in three days, whichever comes first, to ensure that breakthrough volumes are not exceeded. This decision was made from the estimate that the maximum amount of air inhaled by a participant in two minutes would be 40 L. Thus, 400 L for ten participants would be safely below the combined 640 L breakthrough volume established for two charcoal cartridges.

APPENDIX C

BREATH EXPOSURE STUDY ESTABLISHMENT CONSENT FORM

BREATH EXPOSURE STUDY
ESTABLISHMENT CONSENT FORM

The Research Triangle Institute (RTI) is under contract with the U.S. Environmental Protection Agency to develop and test a device which can be used to measure the amounts of volatile organic chemicals inhaled and exhaled by humans. As part of this research contract we would like to evaluate the inhalation of airborne chemicals by people in common environments like homes, stores, vehicles, recreational areas, and the workplace. The data we collect will help us determine if people are exposed to pollutants in these everyday situations and whether breath measurements can be used to estimate these exposures.

We would like to ask you to participate in this research by allowing us to sample the air at your establishment. We wish to emphasize that this is strictly a research project and that RTI will not disclose the identities of participants to anyone, including the contract sponsor. Within RTI knowledge of establishment identities will be strictly limited to the one or two chemists who visit your establishment. The test data which is reported to the EPA and other RTI personnel will be coded to eliminate all participant identities and protect your privacy. Our report to the EPA will include only generic descriptions of establishment types (i.e. hardware store, laundramat, etc.) and not the name or location of specific establishments. Your participation would be strictly voluntary and would not result in disruption of your business operations.

If you agree to participate, a chemist from RTI will collect an initial sample of the air at your establishment for evaluation purposes. This would take approximately 10 to 30 minutes. If specific chemicals are found in this sample then we may ask our chemist to make a return visit and spend up to four hours in your establishment during normal buisiness hours. The chemist would collect an additional air sample during this visit. Several different establishments will be chosen to participate in this final visit. These visits would be carried out between now and May 1989. Results of the analysis at your establishment can be obtained by written request to RTI at the completion of the project in June, 1989.

Your participation in this scientific study is very important in answering questions about human exposure and would be greatly appreciated. If you have any further questions about this research study please call RTI chemist Mr. Kent Thomas at 541-6610 (toll-free from Raleigh, Durham, and Chapel Hill) from 8:30 a.m. to 5:00 p.m. Thank you for your time.

I have read and understand the above statements and do hereby willingly allow RTI to collect air samples at this establishment.

ESTABLISHMENT NAME: ______________________________

MANAGER SIGNATURE: ____________________ DATE: ________

RTI CHEMIST SIGNATURE: ____________________ DATE: ________

APPENDIX D

BREATH AND AIR CONCENTRATION TABLES FOR EXPOSURE EXPERIMENTS

DEFINTIONS OF TERMS

Experiment Title:	Describes whether samples are air, alveolar or whole breath in addition to exposure situation.
Spreadsheet File Name:	Name of Symphony spreadsheet work file where data is stored.
Exposure End Time:	Time at which exposure ended (24 hour clocks, HH;MM).
Compound:	Chemical name of compound measured.
CMPD ID:	EPA identification number for the chemical compound.
Mean Blank:	Mass in blank to be subtracted from measured mass to correct for background. This was not used for this work.
Mean Recov.:	Fractional recovery (1=100%) to correct for incomplete recovery from canister and analysis step. For this work 100% recovery was assumed.
LOD (ng):	Method LOD as described in Section 4.
QL (ng):	Generally, four times the LOD. Measured concentration less than the QL divided by the volume analyzed (in L) are reported as *ND*.
SAMP. ID:	Sample code as defined in QA section.
Volume Analyzed (L):	Volume of sample in liters drawn from the canister and analyzed by GC/MS. For Tenax-based collections, this volume represents the volume of whole breath pulled through the Tenax cartridge.
Real Time (HH:MM):	Time (24 hr clock) at which breath collection was started. The Real Time indicated in the air samples corresponds to the time at which collection terminated.
Elasped Time (Min):	Time in minutes at which the collection of breath was begun minus the time at which the exposure ended.

TABLE D-1

Experiment Title -------> AIR SAMPLES; FURNITURE STRIPPER #1
Spreadsheet File Name---> AIRFS1
Exposure End Time-------> 13:48

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140FS10CF1	SAMP. ID 140FS1ECF1	SAMP. ID 140FS1ECF1	SAMP. ID 140FS1BCF1	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
			VOLUME ANALYZED (L)----->			0.200	0.200	0.020	0.200									
			REAL TIME (HH:MM)------->				13:48	13:48	17:25									
			ELAPSED TIME (MIN) ----->															
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *									
Isopentane 57	45	0.00	1.00	0.06	0.25	5.6	22.9	21.0	5.9									
Pentane 57	46	0.00	1.00	0.07	0.30	5.1	8.7	* ND *	2.4									
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	1.0	* ND *	* ND *									
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	5.5	* ND *	* ND *									
Dichloromethane 84	34	0.00	1.00	0.09	0.34	2.6	NC	5038.6	* ND *									
Chloroform 83	2	0.00	1.00	0.03	0.10	3.5	0.9	* ND *	* ND *									
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	3.2	141.1	120.9	* ND *									
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	0.5	35.9	35.8	1.0									
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *									
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	0.7	38.8	41.6	0.4									
Benzene 78	5	0.00	1.00	0.06	0.24	1.2	2.5	* ND *	1.4									
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	77.4	80.6	* ND *									
Toluene 91	10	0.00	1.00	0.02	0.08	9.2	NC[d]	5679.9	2.8									
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	25.5	18.9	* ND *									
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	8.6	* ND *	* ND *									
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	12.9	* ND *	* ND *									
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	26.0	23.4	* ND *									
Butyl acetate 61 #	62	0.00	1.00	0.02	0.08	* ND *	1.5	* ND *	* ND *									
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	0.4	72.8	59.1	* ND *									
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	0.6	79.2	62.8	0.4									
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	2.3	240.0	238.2	1.7									
n-Nonane 57	33	0.00	1.00	0.02	0.07	0.4	66.4	55.4	* ND *									
Styrene 104	15	0.00	1.00	0.01	0.05	2.0	31.9	22.7	31.9									
o-Xylene 91	21	0.00	1.00	0.02	0.09	0.8	92.1	71.5	0.5									
1,2,4-Trimethylbenzene#	57	0.00	1.00	0.01	0.04	* ND *	2.0	* ND *	* ND *									
n-Decane 57	23	0.00	1.00	0.02	0.12	1.4	136.5	98.5	* ND *									
Trimethylbenzene iso.#	64	0.00	1.00	0.01	0.04	* ND *	3.2	3.0	* ND *									
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	1.7	91.2	74.7	* ND *									
n-Dodecane 57 #	24	0.00	1.00	0.02	0.12	* ND *	15.3	* ND *	* ND *									

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[d] Not calculated because of instrument saturation.

[#] Indicates a non-target compound.

TABLE D-2

Experiment Title -------> ALVEOLAR BREATH CANISTER: FURNITURE STRIPPER #1
Spreadsheet File Name---> ABCFS1
Exposure End Time-------> 13:48

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140FS1ACF0	SAMP. ID 140FS1ACF1	SAMP. ID 140FS1ACF2	SAMP. ID 140FS1ACF3	SAMP. ID 140FS1ACF4	SAMP. ID 140FS1ACF5	SAMP. ID 140FS1ACF6	SAMP. ID 140FS1ACF7	SAMP. ID 140FS1ACF8	SAMP. ID 140FS1ACF9	SAMP. ID 140FS1ACF10	SAMP. ID 140FS1ACF11	SAMP. I
			VOLUME ANALYZED (L)----->			0.058	0.057	0.059	0.060	0.060	0.060	0.060	0.059	0.060	0.059	0.059	0.060	
			REAL TIME (HH:MM)------->			9:57	13:50	13:55	14:05	14:15	14:25	14:41	14:55	15:30	16:00	16:45	17:29	
			ELAPSED TIME (MIN) ----->				2	7	17	27	37	53	67	102	132	177	221	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	45	0.00	1.00	0.06	0.25	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Pentane 57	46	0.30	1.00	0.07	0.30	25.7	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	13.4	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Dichloromethane 84	34	0.00	1.00	0.09	0.34	* ND *	339.1	251.5	193.3	134.4	134.7	105.9	89.1	71.3	55.0	55.0	37.3	
Chloroform 83	2	0.00	1.00	0.03	0.10	3.1	* ND *	* ND *	* ND *	5.7	* ND *	* ND *	* ND *	* ND *	2.5	* ND *	18.5	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	56.3	42.5	34.4	27.0	27.8	24.2	21.1	17.4	14.0	11.4	* ND *	
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	* ND *	4.9	3.4	2.5	1.5	1.7	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	* ND *	5.8	4.2	3.3	2.8	2.3	1.3	* ND *	* ND *	* ND *	* ND *	* ND *	
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	6.8	5.4	4.7	3.2	3.1	2.7	2.7	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	1.5	462.9	350.9	260.9	186.3	190.3	160.8	149.7	133.2	100.5	81.7	39.1	
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	2.3	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	* ND *	3.2	2.4	1.8	1.2	1.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	2.2	1.4	1.4	1.0	0.8	* ND *	* ND *	1.5	* ND *	* ND *	* ND *	
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	* ND *	15.2	5.5	12.2	3.0	2.7	1.9	1.8	4.9	1.1	0.9	1.1	
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	2.2	1.6	1.2	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	1.9	* ND *	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	1.9	* ND *	3.1	* ND *	* ND *	* ND *	* ND *	2.2	* ND *	* ND *	* ND *	
1,2,4-Trimethylbenzene#	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	0.9	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	1.8	* ND *	* ND *	1.7	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	1.7	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	12.8	* ND *	* ND *	* ND *	15.4	* ND *	* ND *	* ND *	

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound.

TABLE D-3

Experiment Title -------> WHOLE BREATH CANISTER; FURNITURE STRIPPER #1
Spreadsheet File Name---> WBCFS1
Exposure End Time-------> 13:48

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140FS1WCF0	SAMP. ID 140FS1WCF1	SAMP. ID 140FS1WCF2	SAMP. ID 140FS1WCF3	SAMP. ID 140FS1WCF4	SAMP. ID 140FS1WCF5	SAMP. ID 140FS1WCD5	SAMP. ID 140FS1WCF6	SAMP. ID 140FS1WCF7	SAMP. ID 140FS1WCF8	SAMP. ID	SAMP. ID	SAMP. ID
			VOLUME ANALYZED (L)----->			0.077	0.079	0.076	0.077	0.080	0.080	0.080	0.080	0.078	0.073			
			REAL TIME (HH:MM)------->			10:04	13:58	14:17	14:34	14:50	15:34	15:34	16:02	16:47	17:31			
			ELAPSED TIME (MIN) ----->				10	29	46	70	106	106	134	179	223			
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Isopentane 57	45	0.00	1.00	0.06	0.25	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Pentane 57	46	0.00	1.00	0.07	0.30	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	*ND*	*ND*	*ND*	*ND*	* ND *	* ND *	* ND *	* ND *	* ND *			
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Dichloromethane 84	34	0.00	1.00	0.09	0.34	* ND *	205.9	144.3	109.6	70.2	56.1	59.2	45.7	55.7	32.9			
Chloroform 83	2	0.00	1.00	0.03	0.10	2.2	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	2.1	1.5	* ND *			
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	30.3	21.9	18.6	12.9	10.1	10.2	8.2	8.4	* ND *			
2-Methylhexane 57#	50	0.00	1.00	0.02	0.07	* ND *	1.9	1.4	1.1	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	* ND *	2.4	1.9	1.7	* ND *	* ND *	* ND *	* ND *	* ND *	1.7			
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	4.6	3.0	2.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Toluene 91	10	0.00	1.00	0.02	0.08	1.7	208.0	198.4	157.0	114.9	93.3	89.3	72.7	56.5	48.8			
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	5.6	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* NC *	* ND *	* ND *	* ND *			
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	* ND *	1.3	1.0	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	1.2	1.3	0.6	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	* ND *	6.3	3.6	2.1	1.6	1.1	1.1	0.9	0.7	0.6			
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	1.4	2.0	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	1.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	1.1	1.6	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	* ND *	1.9	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound.

TABLE D-4

Experiment Title -------> AIR SAMPLES: HARDWARE STORE #1
Spreadsheet File Name---> AIRHS1
Exposure End Time-------> 13:36

						CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]												
COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 14DHS1OCF1	SAMP. ID 14DHS1ECF1	SAMP. ID 14DHS1ECF1	SAMP. ID 14DHS1BCF1	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP
			VOLUME ANALYZED (L)----->			0.200	0.100	0.020	0.200									
			REAL TIME (HH:MM)------->			9:47	13:35	13:35	17:16									
			ELAPSED TIME (MIN) ----->															
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *									
Isopentane 57	45	0.00	1.00	0.06	0.25	61.8	24.0	21.5	30.3									
Pentane 57	46	0.00	1.00	0.07	0.30	24.9	14.2	* ND *	11.7									
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	5.5	7.5	* ND *									
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	9.4	24.1	22.3	5.0									
Dichloromethane 84	34	0.00	1.00	0.09	0.34	17.5	467.2	481.0	* ND *									
Chloroform 83	2	0.00	1.00	0.03	0.10	2.6	* ND *	* ND *	* ND *									
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	341.7	326.6	* ND *									
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	1.6	1.0	13.2	3.0									
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *									
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	2.1	14.3	12.7	2.3									
Benzene 78	5	0.00	1.00	0.06	0.24	2.5	6.6	* ND *	3.3									
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *									
Toluene 91	10	0.00	1.00	0.02	0.08	13.6	339.9	316.1	9.4									
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	39.8	34.7	* ND *									
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *									
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	276.7	260.6	* ND *									
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	25.9	21.4	* ND *									
Butyl acetate 61 #	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *									
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	0.5	95.3	74.2	0.9									
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	0.8	359.1	467.2	1.9									
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	3.1	NC[d]	1612.3	7.1									
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	183.2	161.7	0.4									
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	33.5	32.1	* ND *									
o-Xylene 91	21	0.00	1.00	0.02	0.09	0.8	433.3	435.2	2.4									
1,2,4-Trimethylbenzene#	57	0.00	1.00	0.01	0.04	* ND *	8.3	6.5	* ND *									
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	288.6	265.2	0.7									
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	0.2	19.7	15.0	0.4									
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	0.7	156.7	126.0	0.6									
n-Dodecane 57 #	24	0.00	1.00	0.02	0.10	* ND *	24.4	11.2	* ND *									

[a] All concentrations are to be interpreted only to two significant figures.
[b] Not detected or below QL.
[c] Includes both meta- and para-isomers.
[d] Not calculated because of instrument saturation.
# Indicates a non-target compound.

TABLE D-5

Experiment Title -------> ALVEOLAR BREATH CANISTER; HARDWARE STORE #1
Spreadsheet File Name---> ABCHS1
Exposure End Time-------> 13:36

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 14DHS1ACF0	SAMP. ID 14DHS1ACF1	SAMP. ID 14DHS1ACF2	SAMP. ID 14DHS1ACF3	SAMP. ID 14DHS1ACF4	SAMP. ID 14DHS1ACF5	SAMP. ID 14DHS1ACF6	SAMP. ID 14DHS1ACF7	SAMP. ID 14DHS1ACF8	SAMP. ID 14DHS1ACF9	SAMP. ID 14DHS1ACF10	SAMP. ID 14DHS1ACD10	SAMP. ID[d] 14DHS1ACF11
			VOLUME ANALYZED (L)----->			0.055	0.057	0.060	0.060	0.052	0.053	0.057	0.056	0.056	0.055	0.055	0.053	0.056
			REAL TIME (HH:MM)------->			9:39	13:37	13:41	13:51	14:02	14:13	14:29	14:42	15:10	15:40	16:29	16:29	17:11
			ELAPSED TIME (MIN) ----->				1	5	15	26	37	53	66	94	124	173	173	215
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Isopentane 57	45	0.00	1.00	0.06	0.25	411.1	13.6	10.8	16.1	10.2	7.5	5.3	5.9	* ND *	* ND *	* ND *	* ND *	* ND *
Pentane 57	46	0.00	1.00	0.07	0.30	150.3	7.5	7.2	47.0	8.3	80.4	* ND *	5.0	* ND *	* ND *	9.8	* ND *	* ND *
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	68.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Dichloromethane 84	34	0.00	1.00	0.09	0.34	8.3	71.7	52.0	35.7	25.9	21.9	16.7	14.4	10.0	7.9	6.1	6.5	* ND *
Chloroform 83	2	0.00	1.00	0.03	0.10	2.3	* ND *	* ND *	3.8	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	92.3	70.7	58.5	48.2	41.7	37.7	35.0	28.0	25.2	23.4	23.0	18.6
2-Methylhexane 57	58	0.00	1.00	0.02	0.07	22.1	2.7	2.1	2.6	1.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	10.8	2.8	2.2	-2.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Benzene 78	5	0.00	1.00	0.06	0.24	13.5	4.3	5.4	* ND *	* ND *	4.7	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Toluene 91	10	0.00	1.00	0.02	0.08	14.7	27.8	20.4	17.9	14.4	7.5	6.4	7.3	4.9	4.0	3.6	3.5	2.7
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	2.1	1.3	1.2	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	17.3	49.5	51.7	38.3	36.3	38.1	35.0	29.6	26.6	23.5	22.5	22.3	20.0
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	* ND *	4.4	3.6	2.3	1.5	1.2	* ND *	1.3	* ND *	* ND *	* ND *	* ND *	* ND *
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	19.1	14.4	5.4	4.1	4.0	3.1	4.4	2.1	1.9	1.6	2.0	1.1
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	2.1	48.2	36.7	30.5	25.5	25.0	21.2	21.7	15.3	6.0	5.2	5.6	3.6
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	13.8	5.0	3.6	2.3	1.8	1.4	1.3	* ND *	* ND *	1.4	* ND *	* ND *
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	15.5	12.4	4.2	4.8	3.2	2.5	4.0	1.7	* ND *	* ND *	1.6	* ND *
1,2,4-Trimethylbenzene	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	27.2	15.7	3.9	2.7	2.1	* ND *	1.8	* ND *	* ND *	* ND *	* ND *	* ND *
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	9.4	3.8	2.0	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[d] Not calculated because of instrument saturation.

[#] Indicates a non-target compound.

TABLE D-6

Experiment Title -------> WHOLE BREATH CANISTER; HARDWARE STORE #1
Spreadsheet File Name---> WBCHS1
Exposure End Time-------> 13:36

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140HS1WCF0	SAMP. ID 140HS1WCF1	SAMP. ID 140HS1WCF2	SAMP. ID 140HS1WCF3	SAMP. ID 140HS1WCF4	SAMP. ID 140HS1WCF5	SAMP. ID 140HS1WCD5	SAMP. ID 140HS1WCF6	SAMP. ID 140HS1WCF7	SAMP. ID 140HS1WCF8	SAMP. ID	SAMP. ID	SAMP. ID
VOLUME ANALYZED (L)----->						0.079	0.069	0.071	0.072	0.076	0.077	0.077	0.080	0.079	0.078			
REAL TIME (HH:MM)------->						9:43	13:44	14:05	14:23	14:45	15:12	15:12	15:42	16:33	17:14			
ELAPSED TIME (MIN) ----->							8	29	47	69	96	96	126	177	218			
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Isopentane 57	45	0.00	1.00	0.06	0.25	240.4	10.8	6.7	5.2	4.7	3.2	3.8	3.7	* ND *	3.0			
Pentane 57	46	0.00	1.00	0.07	0.30	89.6	6.9	5.2	4.3	5.1	6.3	5.8	4.2	4.0	4.4			
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	29.3	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Dichloromethane 84	34	0.00	1.00	0.09	0.34	7.2	43.6	23.9	16.9	10.7	8.1	7.9	5.2	4.9	4.8			
Chloroform 83	2	0.00	1.00	0.03	0.10	2.0	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	9.7	51.4	36.9	30.7	23.0	21.4	20.2	14.3	15.8	14.4			
2-Methylhexane 57#	58	0.00	1.00	0.02	0.07	14.0	* ND *	1.2	* ND *	1.0	* ND *	* ND *	* ND *	* ND *	* ND *			
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	*ND*	*ND*	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	6.6	1.7	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Benzene 78	5	0.00	1.00	0.06	0.24	7.3	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Toluene 91	10	0.00	1.00	0.02	0.08	8.0	14.1	8.0	8.1	5.3	5.0	4.6	3.2	2.8	2.7			
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	1.0	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
2-Methylpropyl acetate #	60	0.00	1.00	0.82	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	7.6	36.4	35.0	24.1	21.6	19.1	22.1	14.0	16.8	15.8			
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	* ND *	1.9	2.2	1.4	2.0	* ND *	* ND *	* ND *	* ND *	* ND *			
Ethylbenzene[c] 91	19	0.00	1.00	0.01	0.05	* ND *	6.3	4.0	2.9	2.4	2.0	2.2	1.4	1.2	1.1			
p-Xylene 91	22	0.00	1.00	0.01	0.04	1.4	21.3	13.9	11.3	9.1	7.3	8.5	4.8	4.2	3.6			
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	4.0	2.2	1.6	1.1	1.0	0.9	* ND *	* ND *	* ND *			
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	4.9	2.9	2.4	2.1	1.6	1.7	1.3	* ND *	* ND *			
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	3.7	2.0	1.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[#] Indicates a non-target compound.

TABLE D-7

Experiment Title -------> AIR SAMPLES: SWIMMING POOL #1
Spreadsheet File Name---> AIRSP1
Exposure End Time-------> 11:34

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140SP10CF1	SAMP. ID 140SP1ECF1	SAMP. ID 140SP1BCF1	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
			VOLUME ANALYZED (L)----->			0.060	0.057	0.200										
			REAL TIME (HH:MM)------->			9:15	11:34	15:14										
			ELAPSED TIME (MIN) ----->															
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *										
Isopentane 57	45	0.00	1.00	0.06	0.25	20.3	54.6	40.4										
Pentane 57	46	0.00	1.00	0.07	0.30	15.9	29.7	12.4										
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *										
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	21.7	6.5										
Dichloromethane 84	34	0.00	1.00	0.09	0.34	41.1	* ND *	* ND *										
Chloroform 83	2	0.00	1.00	0.03	0.10	94.4	603.2	1.1										
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	* ND *	* ND *										
2-Methylhexane 57#	58	0.00	1.00	0.02	0.07	2.2	* ND *	1.3										
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *										
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	1.1	16.7	1.7										
Benzene 78	5	0.00	1.00	0.06	0.24	3.7	7.8	2.8										
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* NC *										
Toluene 91	10	0.00	1.00	0.02	0.08	10.7	11.0	7.0										
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	3.8	0.3										
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *										
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *	2.2										
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *										
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *										
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	1.2	5.7	1.3										
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	1.4	1.5	1.2										
p-Xylene[c] 91	22	0.00	1.00	0.01	0.04	7.1	4.7	4.5										
n-Nonane 57	33	0.00	1.00	0.02	0.07	1.5	2.5	1.2										
Styrene 104	15	0.00	1.00	0.01	0.05	1.7	2.8	2.0										
o-Xylene 91	21	0.00	1.00	0.02	0.09	2.0	2.0	1.9										
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *										
n-Decane 57	23	0.00	1.00	0.02	0.10	2.5	9.9	2.0										
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	0.2										
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	10.1	0.9										
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *	3.5										

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[#] Indicates a non-target compound.

TABLE D-8

Experiment Title -------> ALVEOLAR BREATH CANISTER; SWIMMING POOL #1
Spreadsheet File Name---> ABCSP1
Exposure End Time-------> 11:34

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140SP1ACF0	SAMP. ID 140SP1ACF1	SAMP. ID 140SP1ACF2	SAMP. ID 140SP1ACF3	SAMP. ID 140SP1ACF4	SAMP. ID 140SP1ACF5	SAMP. ID 140SP1ACF6	SAMP. ID 140SP1ACD6	SAMP. ID 140SP1ACF7	SAMP. ID 140SP1ACF8	SAMP. ID 140SP1ACF9	SAMP. ID 140SP1ACF10	SAMP. ID
			VOLUME ANALYZED (L)----->			0.058	0.059	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.058	0.059	0.059	
			REAL TIME (HH:MM)------->			9:08	11:36	11:42	11:52	12:02	12:12	12:27	12:27	12:44	13:12	13:42	14:27	
			ELAPSED TIME (MIN) ----->				2	8	18	28	38	53	53	70	98	128	173	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	45	0.00	1.00	0.06	0.25	64.3	22.7	19.2	14.4	7.8	5.7	4.0	3.9	6.9	6.0	7.3	4.4	
Pentane 57	46	0.00	1.00	0.07	0.30	26.6	9.3	9.1	7.7	5.2	* ND *	* ND *	* ND *	* ND *	* ND *	6.2	* ND *	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	8.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Dichloromethane 84	34	0.00	1.00	0.09	0.34	6.4	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Chloroform 83	2	0.00	1.00	0.03	0.10	9.2	81.4	57.1	43.0	39.9	32.8	29.6	27.6	23.2	17.9	16.7	16.1	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylhexane 57[#]	58	0.00	1.00	0.02	0.07	3.5	6.0	4.1	2.4	2.3	1.2	* ND *	1.5	1.1	1.4	1.2	* ND *	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57[#]	59	0.00	1.00	0.02	0.07	2.0	3.1	1.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Benzene 78	5	0.00	1.00	0.06	0.24	4.8	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	3.2	2.0	3.2	1.8	1.9	1.6	1.3	1.6	* ND *	* ND *	1.3	* ND *	
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpropyl acetate[#]	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylcyclohexane (tent.)[#]	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Butyl acetate 61[#]	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57[#]	63	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylbenzene[c] 91	19	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
p-Xylene 91	22	0.00	1.00	0.01	0.04	1.0	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	0.9	* ND *	* ND *	* ND *	* ND *	
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
1,2,4-Trimethylbenzene[#]	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trimethylbenzene iso[#]	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Undecane 57[#]	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Dodecane 57[#]	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[#] Indicates a non-target compound.

TABLE D-9

Experiment Title -------> WOOD SHOP #1; CANISTER AIR SAMPLES
Spreadsheet File Name---> AIPWS1
Exposure End Time-------> 14:02

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140WS10CF1	SAMP. ID 140WS1ECF1	SAMP. ID 140WS1ECD1	SAMP. ID 140WS1BCF1	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
VOLUME ANALYZED (L)----->						0.200	0.050	0.050	0.200									
REAL TIME (HH:MM)------->						9:49	14:02	14:02	17:46									
ELAPSED TIME (MIN) ----->																		
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *									
Isopentane 57	45	0.00	1.00	0.06	0.25	12.1	28.6	30.2	11.8									
Pentane 57	46	0.00	1.00	0.07	0.30	10.4	333.5	342.6	5.8									
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	56.1	55.7	0.7									
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	3.0	29.3	29.3	* ND *									
Dichloromethane 84	34	0.00	1.00	0.09	0.34	1.8	30.8	27.1	5.6									
Chloroform 83	2	0.00	1.00	0.03	0.10	2.1	3.5	3.7	1.7									
1,1,1-Trichloroethane 82	4	0.00	1.00	0.17	0.66	* ND *	16486.5	15514.6	59.9									
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	0.6	6.3	5.9	* ND *									
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	0.9	NC[d]	NC[d]	* ND *									
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	0.4	6.7	6.6	* ND *									
Benzene 78	5	0.00	1.00	0.06	0.24	2.4	6.7	6.7	1.6									
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	14.1	13.5	* ND *									
Toluene 91	10	0.00	1.00	0.02	0.08	17.3	536.8	487.4	8.8									
n-Octane 57	28	0.00	1.00	0.02	0.07	1.0	104.3	106.1	0.8									
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *									
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	37.9	39.9	* ND *									
Ethylcyclohexane (tent.#	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *									
Butyl acetate 61 #	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *									
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	0.5	37.0	33.2	* ND *									
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	1.2	5.1	5.0	0.7									
p-Xylene[c] 91	22	0.00	1.00	0.01	0.04	5.9	17.2	16.6	3.4									
n-Nonane 57	33	0.00	1.00	0.07	0.07	0.8	50.4	53.0	1.4									
Styrene 104	15	0.00	1.00	0.01	0.05	7.4	4.0	3.6	0.9									
o-Xylene 91	21	0.00	1.00	0.02	0.09	2.4	4.4	4.3	0.9									
1,2,4-Trimethylbenzene#	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *									
n-Decane 57	23	0.00	1.00	0.02	0.10	2.0	91.6	80.8	2.5									
Trimethylbenzene iso.#	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *									
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	1.0	8.9	8.8	0.6									
n-Dodecane 57 #	24	0.00	1.00	0.02	0.10	* ND *	1.9	* ND *	* ND *									

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[d] Not calculated; large mass of 1,1,1-trichloroethane might have observed this ion for carbon tetrachloride.

# Indicates a non-target compound.

TABLE D-10

Experiment Title -------> ALVEOLAR BREATH CANISTER: WOOD SHOP #1
Spreadsheet File Name---> ABCWS1
Exposure End Time-------> 14:02

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140WS1ACF0	SAMP. ID 140WS1ACF1	SAMP. ID 140WS1ACF2	SAMP. ID 140WS1ACF3	SAMP. ID 140WS1ACF4	SAMP. ID 140WS1ACF5	SAMP. ID 140WS1ACF6	SAMP. ID 140WS1ACF7	SAMP. ID 140WS1ACF8	SAMP. ID 140WS1ACF9	SAMP. ID 140WS1ACF10	SAMP. ID 140WS1ACF11	SAMP. ID
			VOLUME ANALYZED (L)----->			0.059	0.058	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	
			REAL TIME (HH:MM)------->			9:48	14:05	14:10	14:20	14:30	14:40	14:56	15:11	15:40	16:16	16:58	17:40	
			ELAPSED TIME (MIN) ----->				3	8	18	28	38	54	69	98	134	176	218	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	45	0.00	1.00	0.06	0.25	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Pentane 57	46	0.00	1.00	0.07	0.30	* ND *	15.8	13.3	9.5	7.9	8.5	12.8	6.3	5.0	* ND *	* ND *	* ND *	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	16.0	13.7	9.4	9.6	9.5	8.9	8.2	7.3	6.1	7.1	8.2	
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Dichloromethane 84	34	0.00	1.00	0.09	0.34	* ND *	* ND *	* ND *	* ND *	5.4	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Chloroform 83	2	0.00	1.00	0.03	0.10	2.2	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	6169.4	4605.7	3505.4	2573.5	2955.3	2355.8	1942.6	1689.7	1316.2	1125.7	1040.3	
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	1.3	22.8	18.6	16.1	18.2	14.2	11.9	11.3	5.9	5.5	5.2	4.0	
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	2.2	1.8	1.5	1.5	1.6	1.3	1.1	* ND *	* ND *	* ND *	* ND *	
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	13.8	11.5	10.2	7.6	10.4	6.1	17.6	5.9	5.8	6.1	* ND *	
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Butyl acetate 61 #	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Dodecane 57 #	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	

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[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound.

TABLE D-11

Experiment Title -------> AIR DATA, CONSUMER PRODUCTS #1, TENAX SAMPLES
Spreadsheet File Name---> AIRCP1
Exposure End Time-------> 13:57 5/12/89

CONCENTRATIONS (MICROGRAMS/CUBIC METER)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140CP10TF1	SAMP. ID 140CP1ETF1	SAMP. ID 140CP1ETD1	SAMP. ID 140CP1BTF1	SAMP. ID 140CP1BTF2	SAMP. ID 140CP1BTF3	SAMP. ID 140CP1BTF4	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
			VOLUME ANALYZED (L)----->			14.6	3.1	2.8	11.0	26.2	33.0	25.9						
			START TIME/DATE ----->			20:44 5/11	8:41 5/12	8:41 5/12	14:03 5/12	20:05 5/12	15:28 5/13	15:52 5/14						
			STOP TIME/DATE ----->			7:50 5/12	13:58 5/12	13:58 5/12	20:15 5/12	15:25 5/13	15:50 5/14	10:50 5/15						
n-Octane 71	28	0.00	1.00	5.70	23.00	* ND * [b]	* ND *	* ND *	* ND *	1.2	2.1	2.8						
m,p-Xylene 106	22	0.00	1.00	7.00	28.00	3.4	* ND *	* ND *	3.2	3.4	3.8	5.4						
Styrene 104	15	0.00	1.00	7.00	28.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *						
o-Xylene 106	21	0.00	1.00	6.50	26.00	* ND *	* ND *	* ND *	* ND *	1.1	1.2	1.9						
n-Nonane 128	33	0.00	1.00	6.30	25.00	* ND *	* ND *	* ND *	* ND *	1.2	1.5	1.3						
alpha-Pinene 93	31	0.00	1.00	5.70	23.00	4.2	96.8	92.1	* ND *	4.0	6.0	6.9						
p-Dichlorobenzene 17	17	0.00	1.00	18.00	72.00	* ND *	9354.8	10642.9	217.8	27.1	10.2	5.5						
n-Decane 142	23	0.00	1.00	9.00	36.00	* ND *	* ND *	* ND *	* ND *	* ND *	1.9	* ND *						
Limonene 68	32	0.00	1.00	7.30	29.00	10.1	162.6	154.6	* ND *	6.3	6.2	7.6						
n-Dodecane 170	24	0.00	1.00	9.30	37.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *						

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

TABLE D-12

Experiment Title -------> WHOLE BREATH, CONSUMER PRODUCTS #1, TENAX SAMPLES
Spreadsheet File Name---> WBTCP1A
Exposure End Time-------> 13:57 5/12/89

CONCENTRATIONS (MICROGRAMS/CUBIC METER)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140CP1WTF0	SAMP. ID 140CP1WTF1	SAMP. ID 140CP1WTF2	SAMP. ID 140CP1WTF3	SAMP. ID 140CP1WTF4	SAMP. ID 140CP1WTF5	SAMP. ID 140CP1WTF6	SAMP. ID 140CP1WTF7	SAMP. ID 140CP1WTF8	SAMP. ID 140CP1WTF9	SAMP. ID 140CP1WTF10	SAMP. ID 140CP1WTF11	SAMP. ID 140CP1WTF12
VOLUME ANALYZED (L)----->						18.4	11.8	11.9	11.9	11.9	15.3	16.8	18.3	20.9	17.5	16.0	17.3	16.6
ELAPSED TIME (HRS) ----->							0.05	0.35	0.63	0.95	1.25	1.67	2.17	2.92	3.65	7.22	17.80	30.70
n-Octane 71	28	0.00	1.00	5.70	23.00	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
m,p-Xylene 106	22	0.00	1.00	7.00	28.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Styrene 104	15	0.00	1.00	7.00	28.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
o-Xylene 106	21	0.00	1.00	6.50	26.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
n-Nonane 128	33	0.00	1.00	6.30	25.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
alpha-Pinene 93	31	0.00	1.00	5.70	23.00	* ND *	6.7	3.8	3.1	2.4	2.2	1.7	1.5	1.1	* ND *	* ND *	* ND *	* ND *
p-Dichlorobenzene 17	17	0.00	1.00	18.00	72.00	* ND *	349.6	245.0	209.5	177.6	157.5	137.7	130.2	81.6	102.0	78.2	43.5	34.2
n-Decane 142	23	0.00	1.00	9.00	36.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Limonene 68	32	0.00	1.00	7.30	29.00	7.4	6.4	4.5	4.2	3.4	3.3	2.9	3.3	2.2	2.7	2.8	2.3	6.2
n-Dodecane 170	24	0.00	1.00	9.30	37.00	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

TABLE D-13

Experiment Title -------> WHOLE BREATH, CONSUMER PRODUCTS #1, TENAX SAMPLES, CONTINUED
Spreadsheet File Name---> WBTCP1B
Exposure End Time-------> 13:57 5/12/89

CONCENTRATIONS (MICROGRAMS/CUBIC METER)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140CP1WTF13	SAMP. ID 140CP1WTF14	SAMP. ID	SAMP. ID 140CP1WTD1	SAMP. ID 140CP1WTD3	SAMP. ID 140CP1WTD4	SAMP. ID 140CP1WTD5	SAMP. ID 140CP1WTD6	SAMP. ID 140CP1WTD8	SAMP. ID 140CP1WTD9	SAMP. ID 140CP1WTD11	SAMP. ID 140CP1WTD12	SAMP. ID 140CP1WTD14
VOLUME ANALYZED (L)----->						19.4	15.7		12.2	12.5	12.4	16.3	17.7	22.8	18.7	17.2	17.3	16.3
ELAPSED TIME (HRS) ----->						50.00	68.40		0.05	0.63	0.95	1.25	1.67	2.92	3.65	17.00	30.70	68.40
n-Octane 71	28	0.00	1.00	5.70	23.00	* ND *[b]	* ND *		* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
m,p-Xylene 106	22	0.00	1.00	7.00	28.00	* ND *	1.8		* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	1.9
Styrene 104	15	0.00	1.00	7.00	28.00	* ND *	* ND *		* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
o-Xylene 106	21	0.00	1.00	6.50	26.00	* ND *	* ND *		* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
n-Nonane 128	33	0.00	1.00	6.30	25.00	* ND *	* ND *		* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
alpha-Pinene 93	31	0.00	1.00	5.70	23.00	1.3	* ND *		7.0	3.1	2.6	2.0	1.8	1.3	* ND *	* ND *	1.7	* ND *
p-Dichlorobenzene 17	17	0.00	1.00	18.00	72.00	30.6	22.4		369.1	202.2	175.7	156.7	143.8	83.7	101.2	45.8	35.5	24.7
n-Decane 142	23	0.00	1.00	9.00	36.00	* ND *	* ND *		* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *
Limonene 68	32	0.00	1.00	7.30	29.00	5.7	34.1		7.0	4.3	3.6	3.4	3.3	2.5	2.7	2.5	5.8	36.9
n-Dodecane 170	24	0.00	1.00	9.30	37.00	* ND *	* ND *		* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

TABLE D-14

Experiment Title -------> AIR MONITORING RESULTS FOR GS1 EXPOSURE EXPERIMENT; CANISTER COLLECTION
Spreadsheet File Name---> AIRGS1
Exposure End Time-------> 13:47

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140GS10CF1	SAMP. ID 140GS1ECF1	SAMP. ID 140GS18CF1	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
VOLUME ANALYZED (L)----->						0.200	1.000	0.200										
REAL TIME (HH:MM)------->						11:30	13:47	17:30										
ELAPSED TIME (MIN) ----->																		
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *										
Isopentane 57	45	0.00	1.00	0.06	0.25	32.6	10100.0	15.4										
Pentane 57	46	0.00	1.00	0.07	0.30	35.3	3440.0	5.0										
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *										
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	7.9	1990.0	2.0										
Dichloromethane 84	34	0.00	1.00	0.09	0.34	8.6	* ND *	* ND *										
Chloroform 83	2	0.00	1.00	0.03	0.10	11.5	* ND *	* ND *										
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	6.7	* ND *	* ND *										
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	1.6	342.0	0.6										
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *										
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	2.4	406.0	0.5										
Benzene 78	5	0.00	1.00	0.06	0.24	2.7	427.0	1.2										
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *										
Toluene 91	10	0.00	1.00	0.02	0.08	18.4	1240.0	3.1										
n-Octane 57	28	0.00	1.00	0.02	0.07	0.6	319.0	* ND *										
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *										
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *	* ND *										
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	904.0	* ND *										
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *										
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	1.2		0.8										
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	1.4	2610.0	0.6										
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	5.9	1680.0	1.9										
n-Nonane 57	33	0.00	1.00	0.02	0.07	0.8	12020.0	1.4										
Styrene 104	15	0.00	1.00	0.01	0.05	6.8	* ND *	2.6										
o-Xylene 91	21	0.00	1.00	0.02	0.09	2.5	701.0	0.6										
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	0.2	113.0	* ND *										
n-Decane 57	23	0.00	1.00	0.02	0.10	15.8	13800.0	3.3										
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	0.6	300.0	* ND *										
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	54.5	5590.0	3.4										
n-Dodecane 57 #	24	0.00	1.00	0.02	0.10	0.8	446.0	0.6										

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound.

NOTE: Concentrations for the garage exposure sample (ECF1) were calculated from full scan MS data and relative response factors using a one-point calibration.

TABLE D-15

Experiment Title -------> ALVEOLAR BREATH EXPOSURE EXPERIMENT; GS1 (GARAGE/SOLVENT); CANISTER COLLECTION
Spreadsheet File Name---> ABCGS1
Exposure End Time-------> 13:47

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140GS1ACF0	SAMP. ID 140GS1ACF1	SAMP. ID 140GS1ACF2	SAMP. ID 140GS1ACF3	SAMP. ID 140GS1ACF4	SAMP. ID 140GS1ACF5	SAMP. ID 140GS1ACF6	SAMP. ID 140GS1ACF7	SAMP. ID 140GS1ACF8	SAMP. ID 140GS1ACF9	SAMP. ID 140GS1ACF10	SAMP. ID 140GS1ACF11	SAMP. ID
			VOLUME ANALYZED (L)------>			0.060	0.050	0.060	0.060	0.060	0.060	0.060	0.060	0.059	0.060	0.060	0.060	
			REAL TIME (HH:MM)------->			11:00	13:50	13:55	14:03	14:12	14:29	14:47	15:03	15:34	16:03	16:48	17:34	
			ELAPSED TIME (MIN) ------>				3	8	16	25	42	60	76	107	136	181	227	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	45	0.00	1.00	0.06	0.25	5.6	267.1	160.9	135.0	102.5	76.3	64.0	70.9	64.5	50.0	43.0	32.8	
Pentane 57	46	0.00	1.00	0.07	0.30	7.8	160.3	99.4	84.0	57.2	47.2	42.6	42.6	37.7	29.8	25.6	19.6	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	92.2	80.4	64.2	48.8	33.9	29.3	34.0	22.1	24.7	15.8	16.0	
Dichloromethane 84	36	0.00	1.00	0.09	0.34	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Chloroform 83	2	0.00	1.00	0.03	0.10	3.4	2.8	1.7	1.7	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	1.8	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylhexane 57#	58	0.00	1.00	0.02	0.07	* ND *	81.4	53.3	37.5	27.2	9.8	13.2	14.1	13.6	9.0	7.7	6.5	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	* ND *	48.1	33.2	24.2	17.2	12.3	9.2	9.9	9.1	6.5	5.8	5.0	
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	23.3	16.2	15.8	15.0	9.8	10.0	10.0	9.3	7.8	6.8	5.9	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	2.6	46.7	34.5	33.2	30.4	23.3	22.5	22.7	19.9	17.3	14.9	12.4	
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	8.5	7.4	5.4	4.1	2.9	2.4	2.4	2.3	1.6	1.3	1.2	
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	34.6	27.0	23.4	19.5	13.1	11.1	11.9	9.6	8.8	6.5	5.3	
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	3.8	191.7	146.0	125.0	101.4	71.4	51.6	56.3	18.5	31.9	24.4	20.3	
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	1.3	43.4	35.2	34.0	33.0	26.5	26.3	26.4	24.0	20.6	17.2	14.0	
p-Xylene[c] 91	22	0.00	1.00	0.01	0.04	1.2	32.4	26.5	25.6	23.0	18.4	17.6	18.0	15.5	13.7	6.2	5.0	
n-Nonane 57	33	0.00	1.00	0.02	0.07	6.9	213.7	153.0	157.0	136.4	97.3	89.0	91.0	77.9	60.2	50.0	42.6	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	14.7	11.9	6.6	6.3	4.6	4.1	4.1	3.9	3.0	2.4	2.2	
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	1.9	1.9	1.4	1.6	1.0	0.6	0.9	0.8	0.7	0.7	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	3.3	193.3	149.2	136.5	128.6	92.5	83.2	84.0	78.7	58.3	44.8	38.0	
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	2.6	2.5	2.1	1.8	1.0	0.9	1.2	0.8	* ND *	0.6	* ND *	
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	129.3	77.0	50.6	41.1	28.8	22.0	21.1	17.9	13.5	10.1	9.1	
n-Dodecane 57#	26	0.00	1.00	0.02	0.10	* ND *	9.9	6.3	1.9	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound.

TABLE D-16

Experiment Title -------> WHOLE BREATH EXPOSURE EXPERIMENT: GS1 (GARAGE/FUEL/SOLVENT): CANISTER COLLECTION
Spreadsheet File Name---> WBCGS1
Exposure End Time-------> 13:47

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140GS1WCF0	SAMP. ID 140GS1WCF1	SAMP. ID 140GS1WCF2	SAMP. ID 140GS1WCF3	SAMP. ID 140GS1WCF4	SAMP. ID 140GS1WCD4	SAMP. ID 140GS1WCF5	SAMP. ID 140GS1WCF6	SAMP. ID 140GS1WCF7	SAMP. ID 140GS1WCF8	SAMP. ID	SAMP. ID	SAMP. ID
			VOLUME ANALYZED (L)------>			0.075	0.077	0.074	0.078	0.077	0.076	0.078	0.079	0.078	0.078			
			REAL TIME (HH:MM)------>			11:06	13:59	14:17	14:35	14:56	14:56	15:30	16:07	16:52	17:39			
			ELAPSED TIME (MIN) ----->				12	30	48	69	69	111	140	185	232			
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Isopentane 57	65	0.00	1.00	0.06	0.25	22.0	102.5	123.7	72.2	69.6	66.0	50.6	40.5	30.0	29.3			
Pentane 57	66	0.00	1.00	0.07	0.30	13.1	90.9	69.4	41.0	41.2	37.1	28.3	22.0	19.1	13.7			
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	*ND*	*ND*	*ND*	*ND*	*ND*	*ND*	*ND*	* ND *			
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	69.7	36.0	23.2	21.3	21.9	16.2	12.5	11.0	7.1			
Dichloromethane 84	34	0.00	1.00	0.09	0.34	* ND *	* ND *	* ND *	* ND *	6.5	* ND *	* ND *	* ND *	* ND *	* ND *			
Chloroform 83	2	0.00	1.00	0.03	0.10	3.0	2.0	1.9	1.5	1.4	2.7	1.3	* ND *	1.5	1.5			
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
2-Methylhexane 57#	50	0.00	1.00	0.02	0.07	* ND *	43.0	29.5	17.7	14.5	14.1	10.9	8.6	8.8	5.2			
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	0.9	27.3	19.0	11.5	10.1	10.1	7.7	5.9	6.3	4.0			
Benzene 78	5	0.00	1.00	0.06	0.26	* ND *	23.9	19.0	13.7	12.2	12.2	9.0	7.3	6.2	5.5			
Trichloroethylene 60	7	0.00	1.00	0.06	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Toluene 91	10	0.00	1.00	0.02	0.09	2.3	39.0	32.3	23.5	20.6	20.8	15.6	10.7	8.8	7.5			
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	8.6	5.9	4.9	3.3	4.5	2.1	1.8	1.5	1.4			
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	19.6	15.3	10.3	8.6	8.4	6.6	5.1	4.9	* ND *			
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *			
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	1.8	122.9	101.3	65.0	54.1	54.8	35.1	26.7	26.7	15.9			
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	0.8	37.7	31.1	23.5	20.2	20.3	14.9	11.2	8.5	7.5			
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	0.8	22.9	17.9	13.1	10.4	10.7	7.4	5.9	4.7	4.2			
n-Nonane 57	33	0.00	1.00	0.02	0.07	3.2	231.4	169.1	103.4	82.9	82.1	54.5	41.2	37.4	30.1			
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	1.4	* ND *	* ND *	* ND *	* ND *			
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	8.5	6.8	4.7	4.2	4.3	3.8	2.4	1.9	1.9			
1,2,4-Trimethylbenzene#	57	0.00	1.00	0.01	0.04	* ND *	1.2	1.2	* ND *	0.6	0.6	* ND *	* ND *	* ND *	* ND *			
n-Decane 57	23	0.00	1.00	0.02	0.10	2.1	150.6	120.1	79.6	63.9	62.6	45.6	35.3	28.1	23.1			
Trimethylbenzene iso. #	66	0.00	1.00	0.01	0.04	* ND *	1.3	1.3	0.7	0.7	0.5	* ND *	* ND *	* ND *	* ND *			
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	35.0	23.0	17.3	14.3	14.9	9.1	7.2	6.0	4.9			
n-Dodecane 57#	26	0.00	1.00	0.02	0.10	* ND *	1.0	* ND *	* ND *	* ND *	5.5	* ND *	* ND *	* ND *	* ND *			

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[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound.

TABLE D-17

Experiment Title -------> AIR DATA FOR HARDWARE STORE 2,3: TWO PEOPLE EXPOSED SIMULTANEOUSLY: CANISTER ALVEOLAR BREATH COLLECTIONS*

Spreadsheet File Name---> AIRHS-23

Exposure End Time-------> 11:50

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140HS20CF1	SAMP. ID 140HS3ECD1	SAMP. ID 140HS3ECF1	SAMP. ID 140HS30CF1	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
			VOLUME ANALYZED (L)----->			0.200	0.030	0.030	0.200									
			REAL TIME (HH:MM)------->			00:02	11:50	11:50	00:02									
			ELAPSED TIME (MIN) ----->			\												
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *									
Isopentane 57	45	0.00	1.00	0.06	0.25	25.5	10.6	9.6	21.7									
Pentane 57	46	0.00	1.00	0.07	0.30	15.3	37.6	34.2	12.6									
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	2.2	5.6	5.3	* ND *									
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	5.6	24.7	22.8	0.6									
Dichloromethane 84	34	0.00	1.00	0.09	0.34	652.1	651.9	655.0	1.6									
Chloroform 83	2	0.00	1.00	0.03	0.10	6.3	* ND *	* ND *	12.6									
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	182.6	197.9	199.1	7.0									
2-Methylhexane 57#	58	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *									
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *									
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *									
Benzene 78	5	0.00	1.00	0.06	0.24	1.7	* ND *	* ND *	2.1									
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	1.0									
Toluene 91	10	0.00	1.00	0.02	0.08	6.3	635.2	635.2	10.5									
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	38.2	38.0	0.4									
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *									
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	6.3	16.1	16.0	* ND *									
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *									
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *									
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *									
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	1.6	147.5	146.6	1.3									
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	6.7	560.0	561.9	3.0									
n-Nonane 57	33	0.00	1.00	0.02	0.07	8.0	193.6	210.6	0.7									
Styrene 104	15	0.00	1.00	0.01	0.05	8.9	39.1	37.6	20.6									
o-Xylene 91	21	0.00	1.00	0.02	0.09	1.2	199.1	193.6	1.5									
1,2,4-Trimethylbenzene#	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *									
n-Decane 57	23	0.00	1.00	0.02	0.10	1.0	301.7	360.3	3.3									
Trimethylbenzene iso#	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *									
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *									
n-Dodecane 57#	26	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *									

*Samples 140HS3ECF1 and 140HS3ECD1 represent duplicate samples collected during exposure. Samples 140HS20CF1 and 140HS30CF1 represent overnight, pre-exposure air samples collected by each of the two participants. No sample was collected during breath collection for this experiment because of a sample collection failure.

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

#Indicates a non-target compound not quantitated in this experiment.

TABLE D-18

Experiment Title --------> HARDWARE STORE #2: ALVEOLAR BREATH COLLECTION, CANISTER: TWO PEOPLE EXPOSED SIMULTANEOUSLY
Spreadsheet File Name---> ABCHS2
Exposure End Time--------> 11:50

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 14DHS2ACF0	SAMP. ID 14DHS2ACF1	SAMP. ID 14DHS2ACF2	SAMP. ID 14DHS2ACF3	SAMP. ID 14DHS2ACF4	SAMP. ID 14DHS2ACF5	SAMP. ID 14DHS2ACF6	SAMP. ID 14DHS2ACF7	SAMP. ID 14DHS2ACF8	SAMP. ID 14DHS2ACF9	SAMP. ID 14DHS2ACF10	SAMP. ID 14DHS2ACF11	SAMP. ID
			VOLUME ANALYZED (L)----->			0.060	0.030	0.059	0.059	0.059	0.057	0.059	0.057	0.059	0.060	0.059	0.060	
			REAL TIME (HH:MM)-------->			07:52	11:53	12:00	12:06	12:16	12:26	12:41	12:56	13:26	13:57	14:40	15:28	
			ELAPSED TIME (MIN) ----->				3	10	16	26	36	51	66	96	127	170	218	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	65	0.00	1.00	0.06	0.25	150.9	17.8	6.7	6.3	8.2	12.8	6.7	16.2	6.5	* ND *	* ND *	* ND *	
Pentane 57	44	0.00	1.00	0.07	0.30	70.4	13.3	6.6	8.5	8.5	9.5	7.6	12.6	5.5	5.3	* ND *	* ND *	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpentane 71	67	0.00	1.00	0.08	0.32	36.4	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Dichloromethane 84	36	0.00	1.00	0.09	0.34	41.5	59.2	52.7	67.0	42.7	36.4	29.9	29.9	26.8	28.0	22.1	23.8	
Chloroform 83	2	0.00	1.00	0.03	0.10	3.1	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	1.8	* ND *	3.7	1.6	1.6	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	84.2	126.2	101.5	101.1	95.2	95.3	83.9	94.3	76.5	74.7	68.8	69.0	
2-Methylhexane 57 #	50	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Benzene 78	5	0.00	1.00	0.06	0.24	6.6	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	5.3	38.2	29.6	29.1	24.5	22.1	20.7	24.6	14.6	13.1	9.3	8.3	
n-Octane 57	20	0.00	1.00	0.02	0.07	* ND *	2.6	1.9	2.0	1.6	1.4	1.2	1.3	* ND *	* ND *	* ND *	* ND *	
2-Methylpropyl acetate #	68	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *	6.2	* ND *	6.1	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Butyl acetate 61 #	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	3.7	2.5	2.1	2.0	2.0	1.9	2.1	1.2	1.2	1.1	0.9	
m-Xylene 91[c]	22	0.30	1.00	0.01	0.04	1.1	19.8	13.3	11.7	6.6	6.4	6.1	6.7	3.9	3.7	3.1	2.8	
n-Nonane 57	33	0.00	1.00	0.02	0.07	1.5	10.7	6.9	5.9	5.2	5.3	4.1	4.4	2.9	2.6	2.3	2.2	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	1.0	* ND *	* ND *	0.8	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	3.5	2.4	2.2	2.3	2.0	2.1	2.1	* ND *	* ND *	* ND *	* ND *	
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	20.8	12.6	5.6	5.1	5.1	5.1	4.1	2.1	1.8	* ND *	* ND *	
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Dodecane 57 #	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[#] Indicates a non-target compound not quantitifed in this experiment.

TABLE D-19

Experiment Title -------> HARDWARE STORE #3; ALVEOLAR BREATH COLLECTION, CANISTER; TWO PEOPLE EXPOSED SIMULTANEOUSLY
Spreadsheet File Name---> ABCHS3
Exposure End Time-------> 11:50

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140HS3ACF0	SAMP. ID 140HS3ACF1	SAMP. ID 140HS3ACF2	SAMP. ID 140HS3ACF3	SAMP. ID 140HS3ACF4	SAMP. ID 140HS3ACF5	SAMP. ID 140HS3ACF6	SAMP. ID 140HS3ACF7	SAMP. ID 140HS3ACF8	SAMP. ID 140HS3ACF9	SAMP. ID 140HS3ACF10	SAMP. ID 140HS3ACF11	SAMP. ID
			VOLUME ANALYZED (L)----->			0.060	0.059	0.059	0.058	0.059	0.059	0.059	0.060	0.060	0.060	0.060	0.060	
			REAL TIME (HH:MM)------->			07:52	11:53	12:00	12:06	12:16	12:26	12:41	12:56	13:26	13:57	14:40	15:28	
			ELAPSED TIME (MIN) ----->				3	10	16	26	36	51	66	96	127	170	218	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	45	0.00	1.00	0.06	0.25	65.1	17.5	5.9	4.4	6.3	5.4	6.2	5.7	* ND *	* ND *	* ND *	* ND *	
Pentane 57	46	0.00	1.00	0.07	0.30	36.8	11.4	5.0	* ND *	5.5	* ND *	* ND *	5.5	* ND *	* ND *	* ND *	* ND *	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	*ND*	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	19.2	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Dichloromethane 84	34	0.00	1.00	0.09	0.34	* ND *	24.9	24.0	23.1	20.0	17.9	12.4	12.9	9.5	7.3	5.3	* ND *	
Chloroform 83	2	0.00	1.00	0.03	0.10	2.5	1.8	* ND *	* ND *	1.6	1.7	* ND *	1.7	* ND *	* ND *	* ND *	* ND *	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	51.8	38.5	32.0	27.8	23.2	19.5	17.7	15.5	13.4	11.7	11.5	
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	3.2	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	4.3	33.2	24.6	18.8	20.4	16.4	14.5	13.7	9.7	8.0	6.9	5.5	
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	2.6	1.9	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	5.8	* ND *	* ND *	* ND *	7.2	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	2.7	2.3	1.6	1.9	1.5	1.4	1.1	0.9	0.8	* ND *	* ND *	
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	1.0	14.8	12.1	5.2	6.0	4.9	4.2	3.9	3.0	2.5	2.2	1.6	
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	7.9	6.4	4.0	4.1	3.4	2.9	2.1	1.9	1.4	1.3	1.3	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	2.9	2.3	1.6	1.9	1.5	* ND *	1.4	* ND *	* ND *	* ND *	* ND *	
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	14.9	5.7	4.0	4.1	3.1	3.4	2.0	* ND *	* ND *	* ND *	* ND *	
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound not quantitifed in this experiment.

TABLE D-20

Experiment Title -------> HARDWARE STORE 2 AND 3; DUPLICATE ALVEOLAR CANISTER COLLECTIONS
Spreadsheet File Name---> ABCHS230
Exposure End Time-------> 11:50

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140HS2ACD6	SAMP. ID 140HS2ACD9	SAMP. ID	SAMP. ID 140HS3ACD7	SAMP. ID 140HS3ACD10	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
VOLUME ANALYZED (L)----->						0.058	0.060		0.059	0.058								
REAL TIME (HH:MM)------->						12:41	13:57		12:56	14:40								
ELAPSED TIME (MIN) ----->							127		66	170								
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND * b	* ND *		* ND *	* ND *								
Isopentane 57	45	0.00	1.00	0.06	0.25	7.1	5.7		6.9	* ND *								
Pentane 57	46	0.00	1.00	0.07	0.30	6.2	* ND *		* ND *	* ND *								
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	2.6		* ND *	* ND *								
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	* ND *	* ND *		6.7	* ND *								
Dichloromethane 84	34	0.00	1.00	0.09	0.34	30.0	26.6		12.8	6.3								
Chloroform 83	2	0.00	1.00	0.03	0.10	* ND *	* ND *		1.6	1.8								
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	78.7	73.3		17.7	15.0								
2-Methylhexane 57#	58	0.00	1.00	0.02	0.07	* ND *	* ND *		* ND *	* ND *								
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *		* ND *	* ND *								
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	* ND *	* ND *		* ND *	* ND *								
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	* ND *		* ND *	* ND *								
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *		* ND *	* ND *								
Toluene 91	10	0.00	1.00	0.02	0.08	18.2	12.6		14.5	6.8								
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	* ND *		* ND *	* ND *								
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *		* ND *	* ND *								
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	* ND *		* ND *	* ND *								
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	* ND *		* ND *	* ND *								
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *		* ND *	* ND *								
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	* ND *	* ND *		* ND *	* ND *								
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	1.6	1.3		1.2	* ND *								
p-Xylene 91 [c]	22	0.00	1.00	0.01	0.04	5.3	3.6		3.9	2.1								
n-Nonane 57	33	0.00	1.00	0.02	0.07	3.7	2.6		3.2	1.3								
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *		* ND *	* ND *								
o-Xylene 91	21	0.00	1.00	0.02	0.09	1.7	* ND *		1.5	* ND *								
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *		* ND *	* ND *								
n-Decane 57	23	0.00	1.00	0.02	0.10	3.4	1.7		2.1	* ND *								
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *		* ND *	* ND *								
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	* ND *		* ND *	* ND *								
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *		* ND *	* ND *								

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[#] Indicates a non-target compound not quantitifed in this experiment.

TABLE D-21

Experiment Title -------> HARDWARE STORE 4.5: CANISTER AIR DATA
Spreadsheet File Name---> AIRHS45
Exposure End Time-------> 12:13

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 14DHS40CF1	SAMP. ID 14DHS50CF1	SAMP. ID	SAMP. ID 14DHS4ECF1	SAMP. ID 14DHS5ECF1	SAMP. ID	SAMP. ID 14DHS4BCF1	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
VOLUME ANALYZED (L)----->						0.200	0.200		0.050	0.050		0.200						
REAL TIME (HH:MM)------->						8:18	8:18		12:13	12:13		15:56						
ELAPSED TIME (MIN) ----->																		
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *		* ND *	* ND *		* ND *						
Isopentane 57	45	0.00	1.00	0.06	0.25	13.0	21.3		7.0	6.3		8.5						
Pentane 57	46	0.00	1.00	0.07	0.30	4.9	10.3		13.6	12.4		2.9						
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	1.7	* ND *		5.0	3.1		* ND *						
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	2.7	3.9		14.2	10.6		2.0						
Dichloromethane 84	34	0.00	1.00	0.09	0.34	28.5	17.1		320.6	218.0		* ND *						
Chloroform 83	2	0.00	1.00	0.03	0.10	5.6	5.3		4.6	3.8		* ND *						
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	135.1	* ND *		225.4	201.5		* ND *						
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	* ND *	* ND *		* ND *	* ND *		* ND *						
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *		* ND *	* ND *		* ND *						
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	* ND *	* ND *		* ND *	* ND *		* ND *						
Benzene 78	5	0.00	1.00	0.06	0.24	1.7	1.8		6.4	* ND *		1.4						
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	1.3		* ND *	* ND *		* ND *						
Toluene 91	10	0.00	1.00	0.02	0.08	41.5	56.3		456.2	282.2		7.3						
n-Octane 57	28	0.00	1.00	0.02	0.07	10.3	0.5		33.0	23.1		0.5						
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	* ND *		* ND *	* ND *		* ND *						
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	4.2	* ND *		185.1	154.5		3.0						
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32	* ND *	* ND *		* ND *	* ND *		* ND *						
Butyl acetate 61#	62	0.00	1.00	0.02	0.08	* ND *	* ND *		* ND *	* ND *		* ND *						
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	* ND *	* ND *		* ND *	* ND *		* ND *						
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	1.6	1.3		57.2	37.7		1.3						
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	5.5	4.7		234.5	155.0		5.8						
n-Nonane 57	33	0.00	1.00	0.02	0.07	3.2	1.0		125.0	107.2		2.5						
Styrene 104	15	0.00	1.00	0.01	0.05	6.6	1.1		18.7	13.8		1.2						
o-Xylene 91	21	0.00	1.00	0.02	0.09	1.6	1.7		101.1	66.1		2.4						
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *		* ND *	* ND *		* ND *						
n-Decane 57	23	0.00	1.00	0.02	0.10	5.5	1.1		212.5	169.5		9.9						
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *		* ND *	* ND *		* ND *						
n-Undecane 57#	29	0.00	1.00	0.02	0.10	* ND *	* ND *		* ND *	* ND *		* ND *						
n-Dodecane 57#	24	0.00	1.00	0.02	0.10	* ND *	* ND *		* ND *	* ND *		* ND *						

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[#] Indicates a non-target compound not quantitifed in this experiment.

TABLE D-22

Experiment Title -------> Hardware Store #4; canister collection of Alveolar Breath
Spreadsheet File Name---> ABCHS4
Exposure End Time-------> 12:13

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140HS4ACF0	SAMP. ID 140HS4ACF1	SAMP. ID 140HS4ACF2	SAMP. ID 140HS4ACF3	SAMP. ID 140HS4ACF4	SAMP. ID 140HS4ACF5	SAMP. ID 140HS4ACF6	SAMP. ID 140HS4ACF7	SAMP. ID 140HS4ACF8	SAMP. ID 140HS4ACF9	SAMP. ID 140HS4ACF10	SAMP. ID 140HS4ACF11	SAMP. ID
			VOLUME ANALYZED (L)----->			0.058	0.059	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.059	0.058	
			REAL TIME (HH:MM)------->			8:06	12:16	12:23	12:31	12:41	12:51	13:06	13:22	13:51	14:23	15:06	15:52	
			ELAPSED TIME (MIN) ----->				3	10	18	28	38	53	69	98	130	173	219	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	45	0.00	1.00	0.06	0.25	62.9	* ND *	4.0	4.0	* ND *	* ND *	3.9	6.5	* ND *	* ND *	* ND *	* ND *	
Pentane 57	46	0.00	1.00	0.07	0.30	27.8	9.0	* ND *	* ND *	9.7	* ND *	* ND *	4.6	* ND *	* ND *	* ND *	* ND *	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	3.8	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	12.1	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Dichloromethane 84	34	0.00	1.00	0.09	0.34	* ND *	48.5	34.5	28.6	26.0	21.4	17.7	14.7	13.0	* ND *	9.2	6.2	
Chloroform 83	2	0.00	1.00	0.03	0.10	5.5	4.5	2.2	3.1	2.4	2.3	3.1	2.8	2.7	1.8	2.1	3.0	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	45.5	90.5	58.5	54.2	50.2	47.2	43.1	42.0	38.8	37.7	38.7	46.3	
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	3.9	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	3.7	55.7	26.8	24.4	21.1	19.3	18.5	15.6	14.3	13.2	12.4	15.0	
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	5.0	2.2	1.9	1.6	1.3	1.5	1.3	2.8	* ND *	* ND *	1.3	
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	66.9	46.1	39.7	34.8	31.9	25.1	20.4	15.6	14.2	12.4	12.3	
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Butyl acetate 61 #	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	3.2	1.3	1.2	0.8	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	* ND *	18.4	4.4	4.1	2.9	2.5	2.5	2.8	1.7	1.4	1.4	1.9	
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	18.9	6.8	6.3	4.6	4.1	3.8	2.7	2.3	1.9	1.9	2.2	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	3.9	1.4	1.4	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
1,2,4-Trimethylbenzene#	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	31.4	16.2	14.7	12.6	4.4	4.2	3.0	2.3	2.2	1.6	2.2	
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Dodecane 57 #	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

# Indicates a non-target compound not quantitifed in this experiment.

TABLE D-23

Experiment Title -------> HARDWARE STORE #5: CANISTER COLLECTION OF ALVEOLAR BREATH
Spreadsheet File Name---> ABCHS5
Exposure End Time-------> 12:13

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID 140HS5ACF0	SAMP. ID 140HS5ACF1	SAMP. ID 140HS5ACF2	SAMP. ID 140HS5ACF3	SAMP. ID 140HS5ACF4	SAMP. ID 140HS5ACF5	SAMP. ID 140HS5ACF6	SAMP. ID 140HS5ACF7	SAMP. ID 140HS5ACF8	SAMP. ID 140HS5ACF9	SAMP. ID 140HS5ACF10	SAMP. ID 140HS5ACF11	SAMP. ID
VOLUME ANALYZED (L)----->						0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	0.060	
REAL TIME (HH:MM)------->						8:06	12:16	12:23	12:31	12:41	12:51	13:06	13:22	13:51	14:23	15:06	15:52	
ELAPSED TIME (MIN) ----->							3	10	18	28	38	53	69	98	130	173	219	
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27	* ND *[b]	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Isopentane 57	45	0.00	1.00	0.06	0.25	217.2	16.5	27.2	10.2	15.6	13.9	14.3	9.0	* ND *	4.6	7.3	9.0	
Pentane 57	46	0.00	1.00	0.07	0.30	81.2	7.9	15.3	5.8	9.0	6.2	6.4	4.7	* ND *	* ND *	* ND *	4.8	
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13	* ND *	*ND*	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpentane 71	47	0.00	1.00	0.08	0.32	41.8	* ND *	5.5	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Dichloromethane 84	34	0.00	1.00	0.09	0.34	* ND *	23.5	20.2	24.3	19.2	14.4	16.3	16.0	13.5	10.5	7.4	5.7	
Chloroform 83	2	0.00	1.00	0.03	0.10	1.9	2.2	1.6	2.3	2.2	2.0	2.2	2.4	2.1	1.9	* ND *	1.7	
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66	* ND *	32.4	22.0	29.6	21.7	18.5	20.2	20.3	18.8	16.8	14.5	15.1	
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methylhexane 57#	59	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Benzene 78	5	0.00	1.00	0.06	0.24	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Trichloroethylene 60	7	0.00	1.00	0.04	0.17	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Toluene 91	10	0.00	1.00	0.02	0.08	6.7	26.9	16.6	17.6	13.7	13.6	15.3	15.4	11.5	6.8	5.5	7.4	
n-Octane 57	28	0.00	1.00	0.02	0.07	* ND *	1.1	* ND *	1.3	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
2-Methylpropyl acetate #	60	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36	* ND *	32.5	16.8	23.1	15.7	11.8	15.2	13.4	10.5	11.0	11.3	12.1	
Ethylcyclohexane (tent.)#	61	0.00	1.00	0.08	0.32	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Butyl acetate 61 #	62	0.00	1.00	0.02	0.08	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
3-Methyloctane 57#	63	0.00	1.00	0.02	0.07	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
Ethylbenzene 91	19	0.00	1.00	0.01	0.05	* ND *	1.5	1.1	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04	1.2	5.4	3.5	2.1	1.7	2.0	2.2	1.1	1.0	0.9	0.7	1.0	
n-Nonane 57	33	0.00	1.00	0.02	0.07	* ND *	4.1	2.7	3.0	1.9	1.6	1.9	1.2	* ND *	* ND *	* ND *	* ND *	
Styrene 104	15	0.00	1.00	0.01	0.05	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
o-Xylene 91	21	0.00	1.00	0.02	0.09	* ND *	1.8	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Decane 57	23	0.00	1.00	0.02	0.10	* ND *	14.0	4.8	3.1	2.3	1.9	2.9	1.6	* ND *	* ND *	* ND *	* ND *	
Trimethylbenzene iso.#	64	0.00	1.00	0.01	0.04	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Undecane 57 #	29	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	
n-Dodecane 57 #	24	0.00	1.00	0.02	0.10	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	* ND *	

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

#Indicates a non-target compound not quantitifed in this experiment.

TABLE D-24

Experiment Title -------> HARDWARE STORE 4,5; ALVEOLAR BREATH, CANISTER COLLECTION DUPLICATES
Spreadsheet File Name---> ABCHS450
Exposure End Time-------> 12:13

CONCENTRATIONS (MICROGRAMS/CUBIC METER @ 25 deg. C; 1 atm.)[a]

COMPOUND	CMPD. ID	Mean Blank	Mean Recov.	LOD (NG)	QL (NG)	SAMP. ID	SAMP. ID 140HS5ACD1	SAMP. ID 140HS5ACD2	SAMP. ID	SAMP. ID 140HS4ACD7	SAMP. ID 140HS4ACD8	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID	SAMP. ID
			VOLUME ANALYZED (L)----->				0.060	0.060		0.060	0.060							
			REAL TIME (HH:MM)------->				12:16	12:23		13:22	13:51							
			ELAPSED TIME (MIN) ----->				3	10		69	98							
Vinyl Chloride 62	36	0.00	1.00	0.07	0.27		* ND *[b]	* ND *		* ND *	* ND *							
Isopentane 57	45	0.00	1.00	0.06	0.25		16.5	25.3		5.4	* ND *							
Pentane 57	46	0.00	1.00	0.07	0.30		7.7	11.8		* ND *	* ND *							
Vinylidene Chloride 61	1	0.00	1.00	0.03	0.13		* ND *	* ND *		* ND *	* ND *							
2-Methylpentane 71	47	0.00	1.00	0.08	0.32		* ND *	5.0		* ND *	* ND *							
Dichloromethane 84	34	0.00	1.00	0.09	0.34		27.5	20.5		14.0	12.4							
Chloroform 83	2	0.00	1.00	0.03	0.10		1.8	* ND *		2.1	2.0							
1,1,1-Trichloroethane 61	4	0.00	1.00	0.17	0.66		36.2	22.6		41.9	38.1							
2-Methylhexane 57 #	58	0.00	1.00	0.02	0.07		* ND *	* ND *		* ND *	* ND *							
Carbon Tetrachloride 82	6	0.00	1.00	0.02	0.10		* ND *	* ND *		* ND *	* ND *							
3-Methylhexane 57 #	59	0.00	1.00	0.02	0.07		* ND *	* ND *		* ND *	* ND *							
Benzene 78	5	0.00	1.00	0.06	0.24		* ND *	* ND *		* ND *	* ND *							
Trichloroethylene 60	7	0.00	1.00	0.04	0.17		* ND *	* ND *		* ND *	* ND *							
Toluene 91	10	0.00	1.00	0.02	0.08		23.5	15.7		14.7	14.1							
n-Octane 57	28	0.00	1.00	0.02	0.07		2.0	* ND *		* ND *	* ND *							
2-Methylpropyl acetate#	60	0.00	1.00	0.02	0.08		* ND *	* ND *		* ND *	* ND *							
Tetrachloroethylene 59	11	0.00	1.00	0.09	0.36		31.8	17.7		20.4	16.4							
Ethylcyclohexane (tent.) #	61	0.00	1.00	0.08	0.32		* ND *	* ND *		* ND *	* ND *							
Butyl acetate 61#	62	0.00	1.00	0.02	0.08		* ND *	* ND *		* ND *	* ND *							
3-Methyloctane 57 #	63	0.00	1.00	0.02	0.07		* ND *	* ND *		* ND *	* ND *							
Ethylbenzene 91	19	0.00	1.00	0.01	0.05		1.3	0.9		* ND *	* ND *							
p-Xylene 91[c]	22	0.00	1.00	0.01	0.04		5.8	3.1		2.0	1.9							
n-Nonane 57	33	0.00	1.00	0.02	0.07		4.7	2.5		2.8	2.2							
Styrene 104	15	0.00	1.00	0.01	0.05		* ND *	* ND *		* ND *	* ND *							
o-Xylene 91	21	0.00	1.00	0.02	0.09		1.8	* ND *		* ND *	* ND *							
1,2,4-Trimethylbenzene #	57	0.00	1.00	0.01	0.04		* ND *	* ND *		* ND *	* ND *							
n-Decane 57	23	0.00	1.00	0.02	0.10		14.5	3.1		2.9	2.2							
Trimethylbenzene iso. #	64	0.00	1.00	0.01	0.04		* ND *	* ND *		* ND *	* ND *							
n-Undecane 57#	29	0.00	1.00	0.02	0.10		* ND *	* ND *		* ND *	* ND *							
n-Dodecane 57#	24	0.00	1.00	0.02	0.10		* ND *	* ND *		* ND *	* ND *							

[a] All concentrations are to be interpreted only to two significant figures.

[b] Not detected or below QL.

[c] Includes both meta- and para-isomers.

[#] Indicates a non-target compound not quantitifed in this experiment.

APPENDIX E

DECAY DATA IN GRAPHICAL FORM

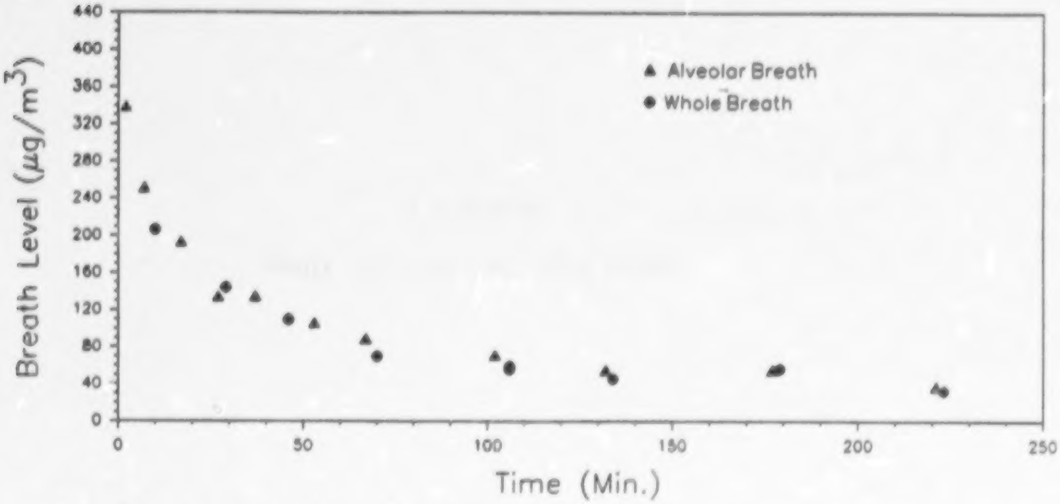

Figure E-1. Breath level of dichloromethane post exposure to furniture stripping operations. Exposure: 5000 $\mu g/m^3$; QL = 6 $\mu g/m^3$.

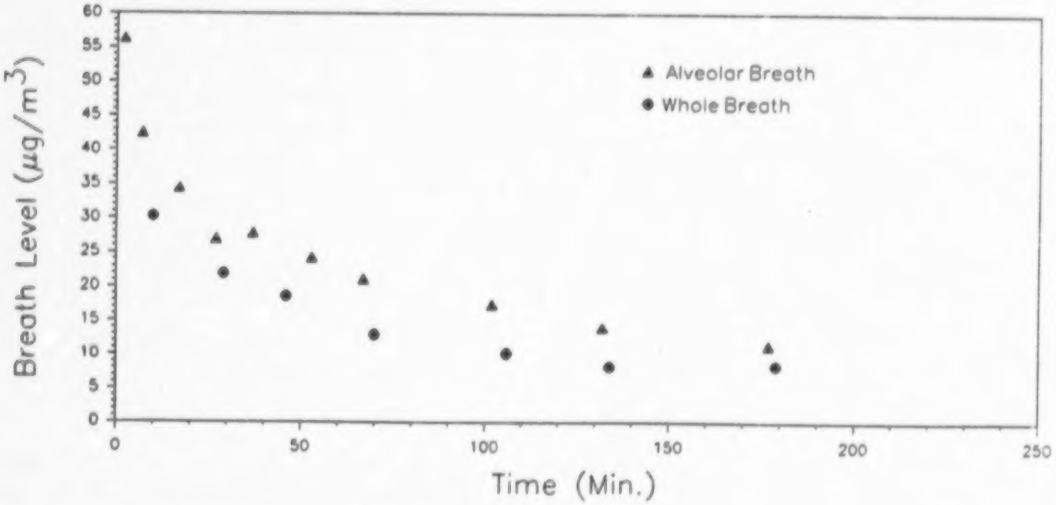

Figure E-2. Breath level of 1,1,1-trichloroethane post exposure to furniture stripping operations. Exposure: 120 $\mu g/m^3$; QL = 8 $\mu g/m^3$.

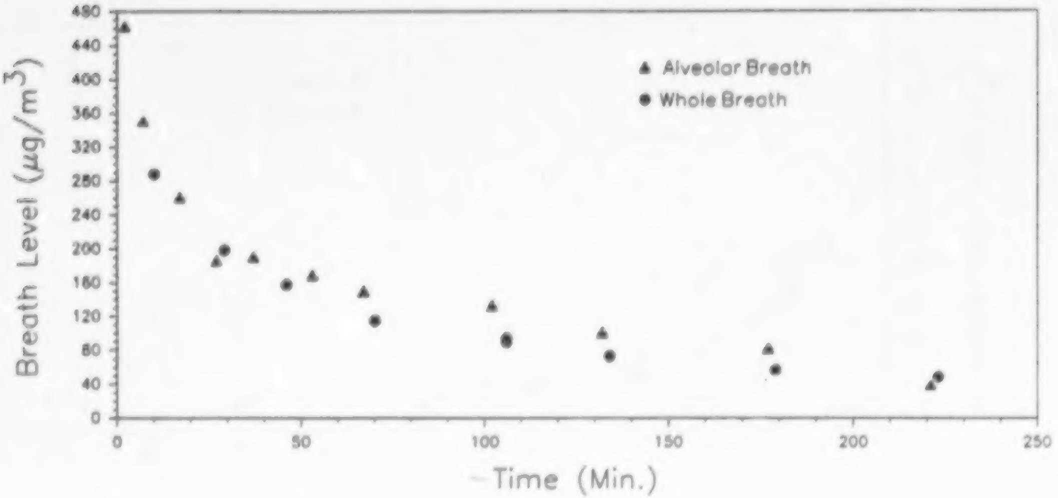

Figure E-3. Breath level of toluene post exposure to furniture stripping operations. Exposure: 5700 μg/m³; QL = 1.4 μg/m³.

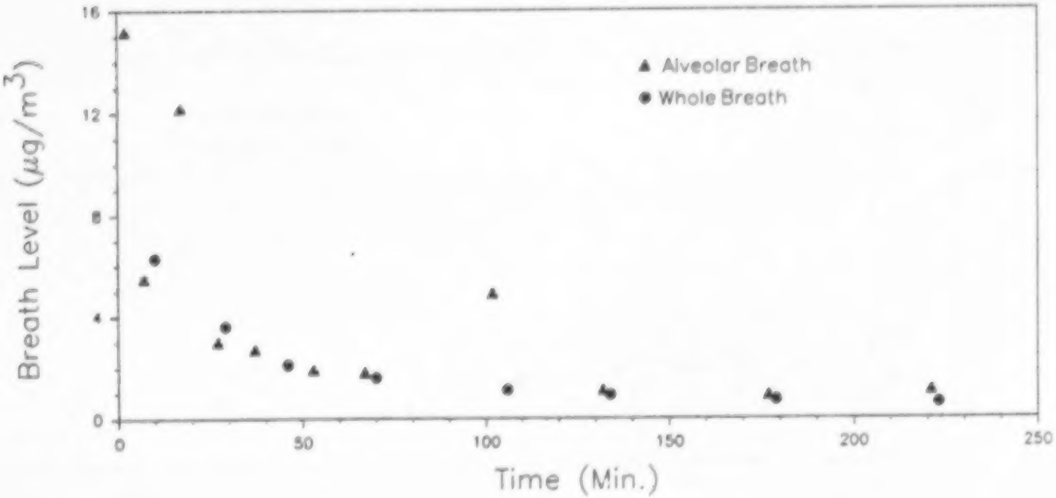

Figure E-4. Breath level of p-xylene post exposure to furniture stripping operations. Exposure: 240 μg/m³; QL = 0.7 μg/m³.

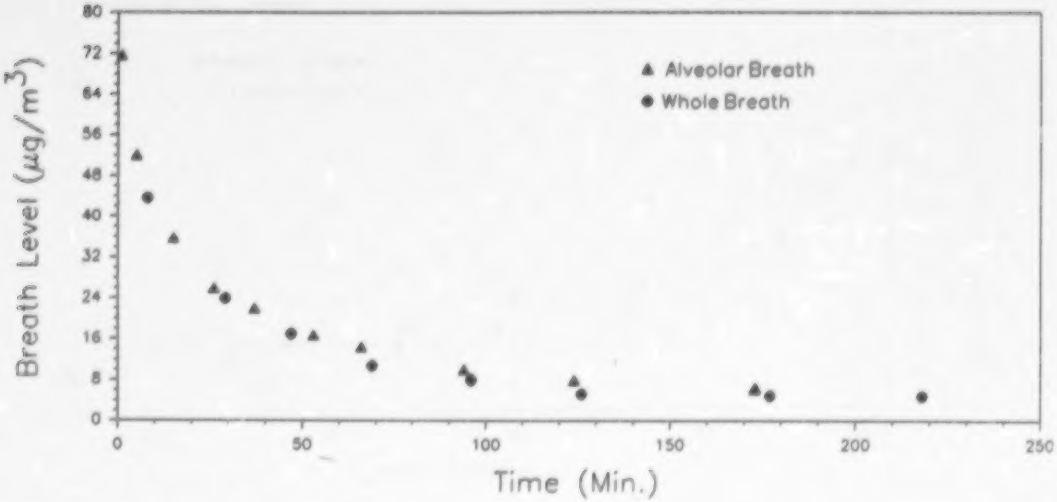

Figure E-5. Breath level of dichloromethane post exposure to hardware store environment. Exposure: 480 $\mu g/m^3$; QL = 0.4 $\mu g/m^3$.

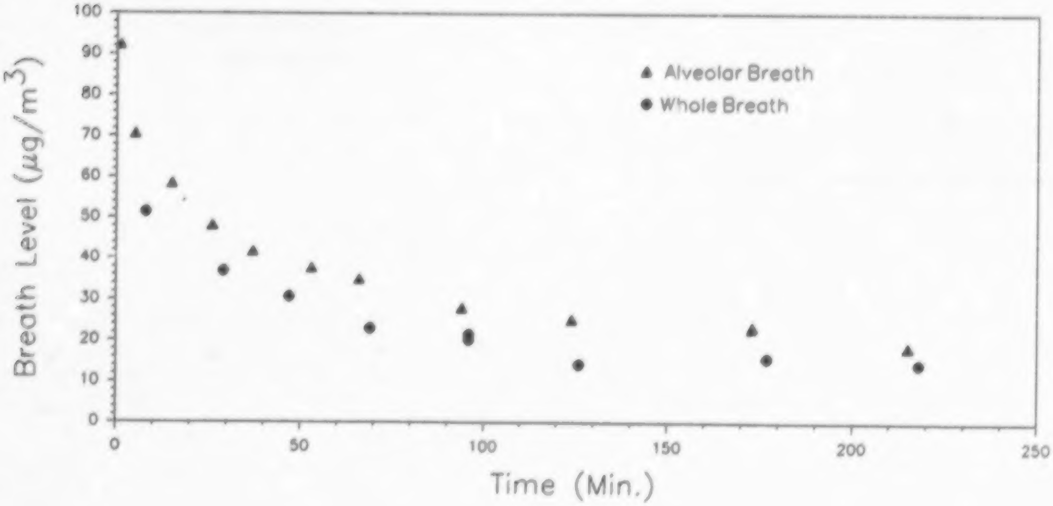

Figure E-6. Breath level of 1,1,1-trichloroethane post exposure to hardware store environment. Exposure: 330 $\mu g/m^3$; QL = 8 $\mu g/m^3$.

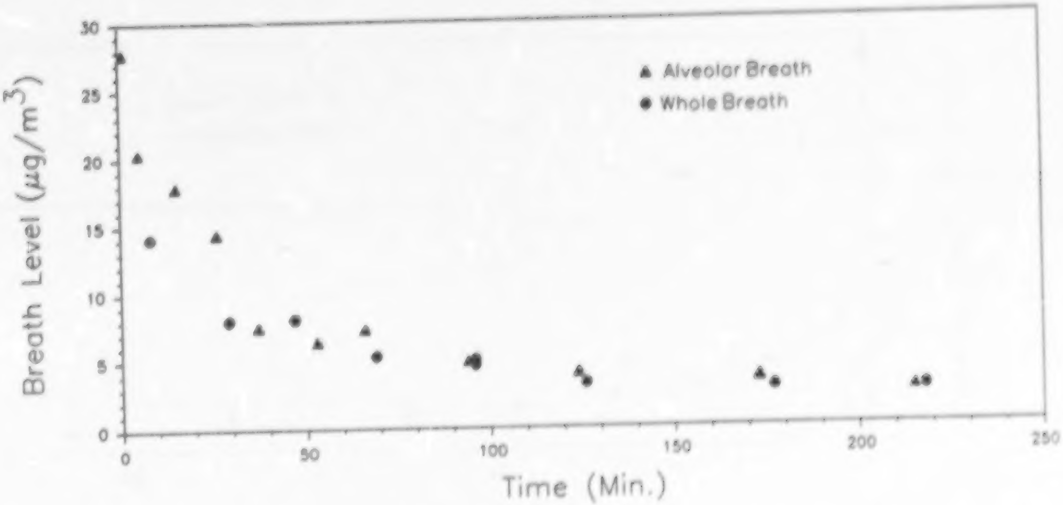

Figure E-7. Breath level of toluene post exposure to hardware store environment. Exposure: 320 µg/m^3; QL = 1.4 µg/m^3.

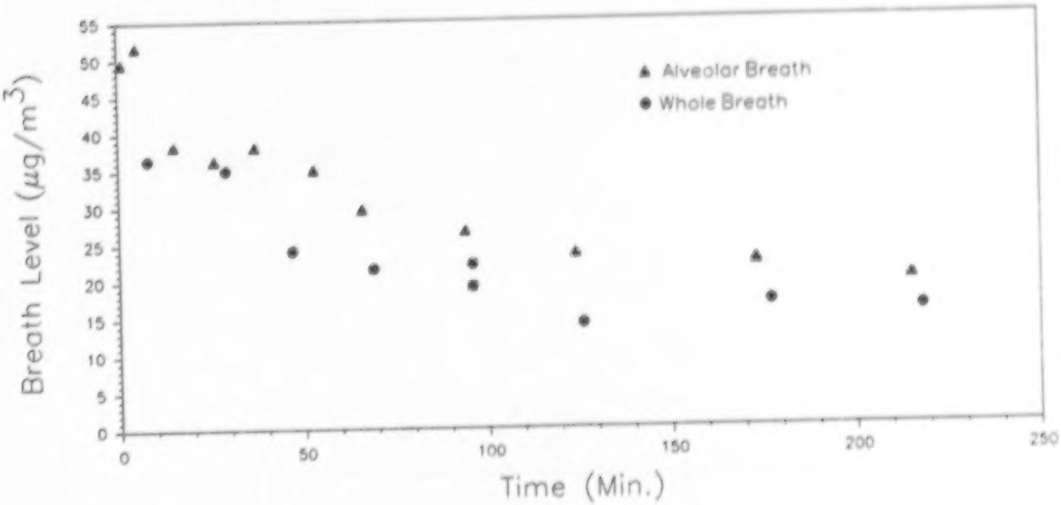

Figure E-8. Breath level of tetrachloroethylene post exposure to hardware store environment. Exposure: 260 µg/m^3; QL = 6.3 µg/m^3.

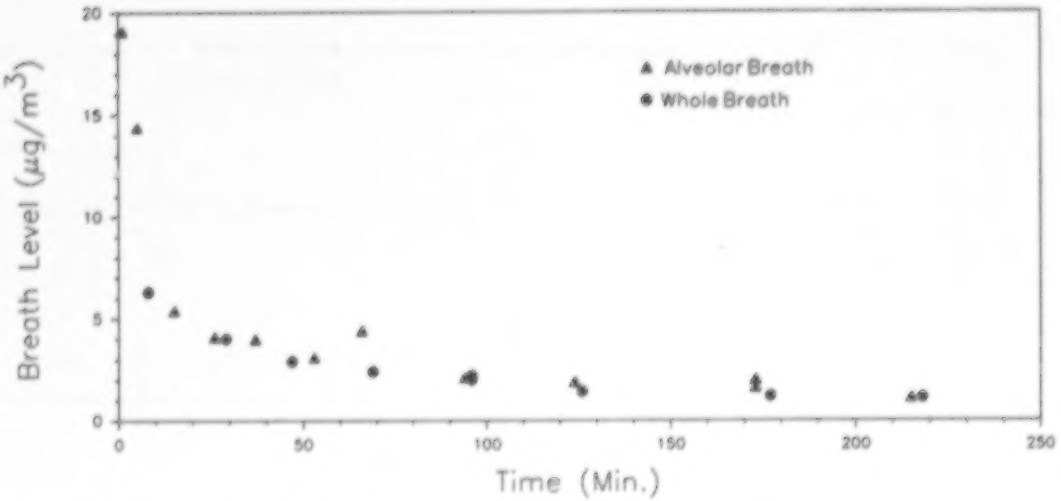

Figure E-9. Breath level of ethylbenzene post exposure to hardware store environment. Exposure: 470 µg/m³; QL = 0.9 µg/m³.

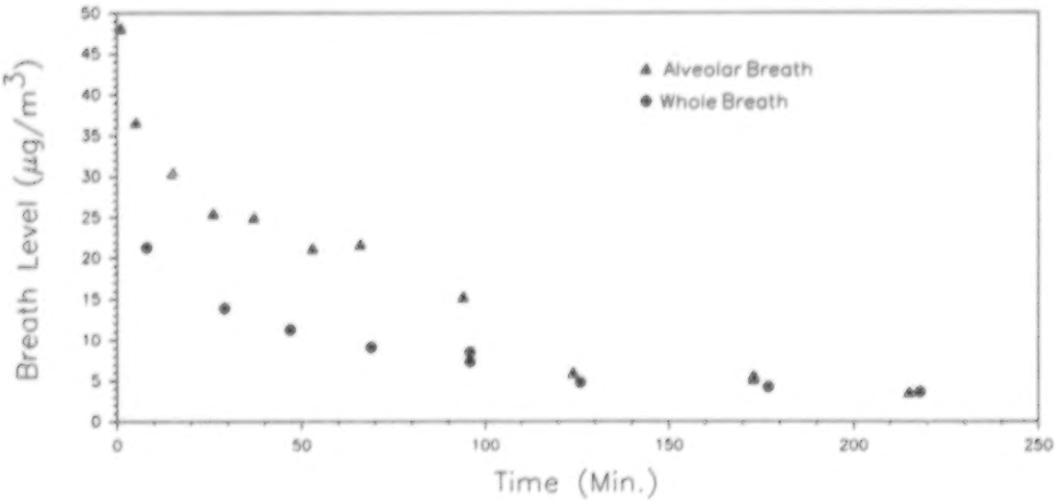

Figure E-10. Breath level of p-xylene post exposure to hardware store environment. Exposure: 1600 µg/m³; QL = 0.7 µg/m³.

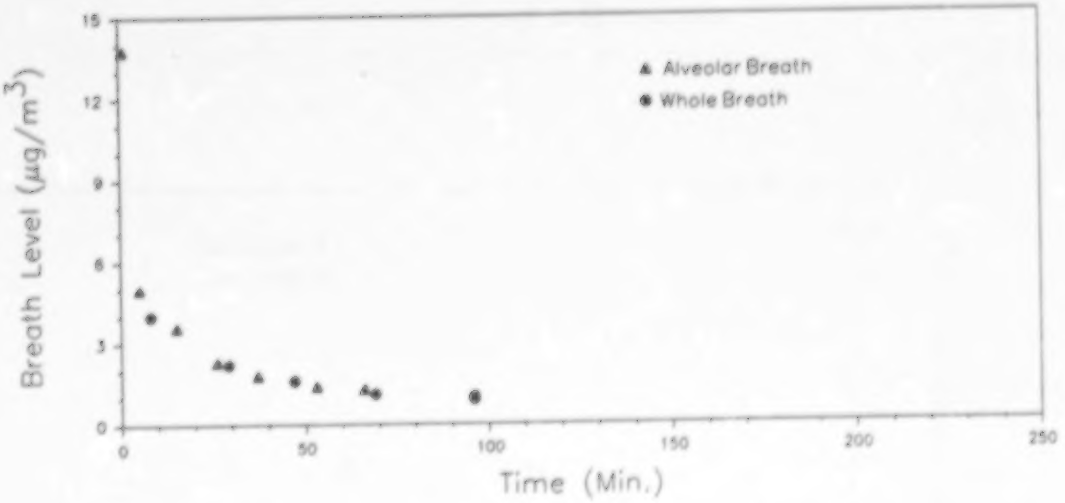

Figure E-11. Breath level of n-nonane post exposure to hardware store environment. Exposure: 160 µg/m^3; QL = 0.9 µg/m^3.

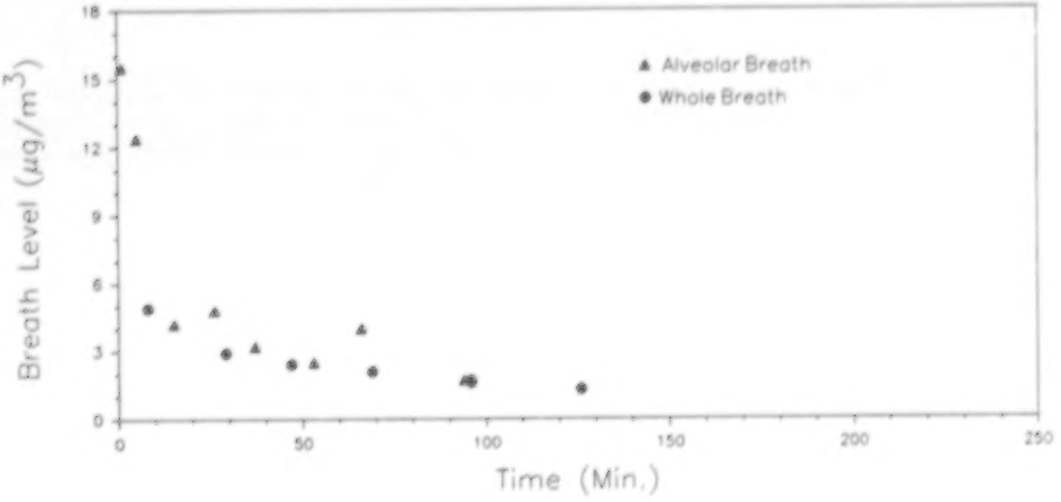

Figure E-12. Breath level of o-xylene post exposure to hardware store environment. Exposure: 440 µg/m^3; QL = 1.1 µg/m^3.

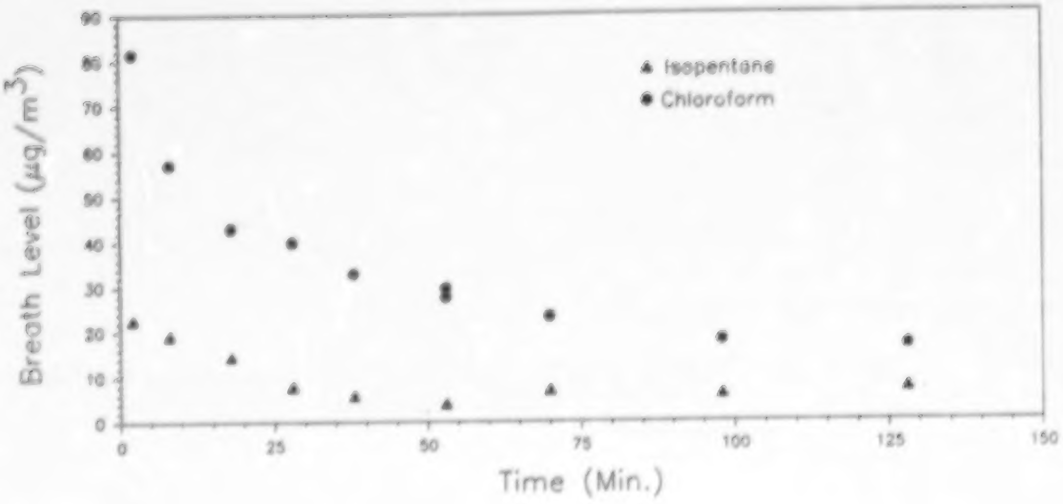

Figure E-13. Decay of isopentane and chloroform in alveolar breath after exposure to an indoor swimming pool. Isopentane exposure: 55 $\mu g/m^3$, QL = 4 $\mu g/m^3$; chloroform exposure: 600 $\mu g/m^3$; QL = 1.7 $\mu g/m^3$.

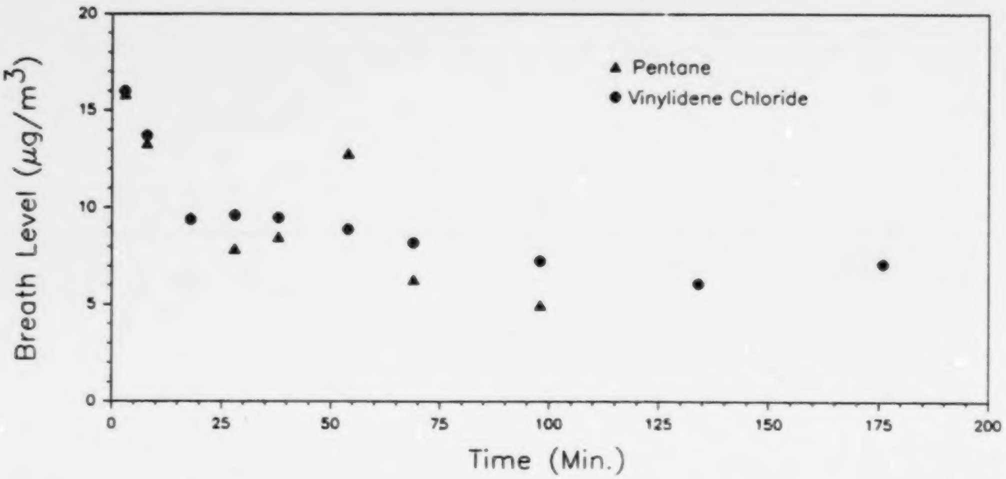

Figure E-14. Decay of pentane and vinylidene chloride in alveolar breath after exposure to an active wood working and metal shop. Pentane exposure: 440 µg/m^3, QL = 5.3 µg/m^3; vinylidene chloride exposure: 56 µg/m^3; QL = 2.3 µg/m^3.

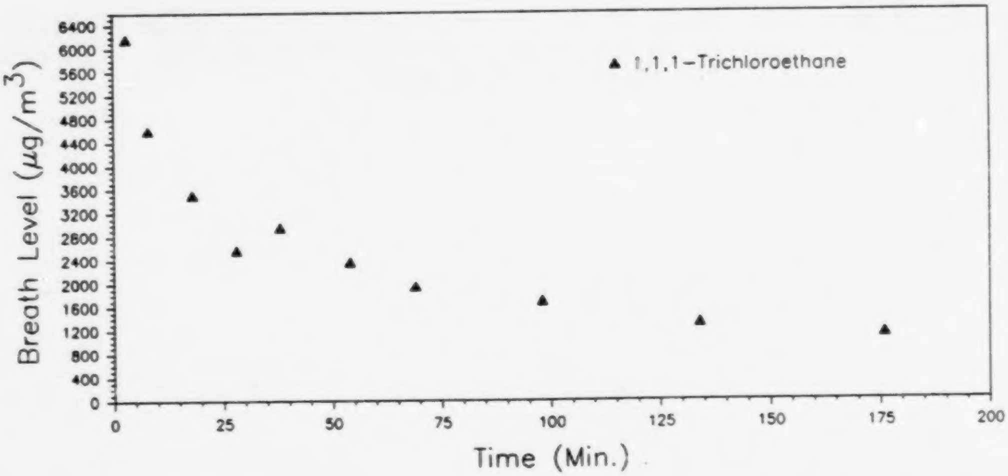

Figure E-15. Decay of 1,1,1-trichloroethane in alveolar breath after exposure to an active wood working and metal shop. Exposure: 16000 µg/m^3; QL = 12 µg/m^3.

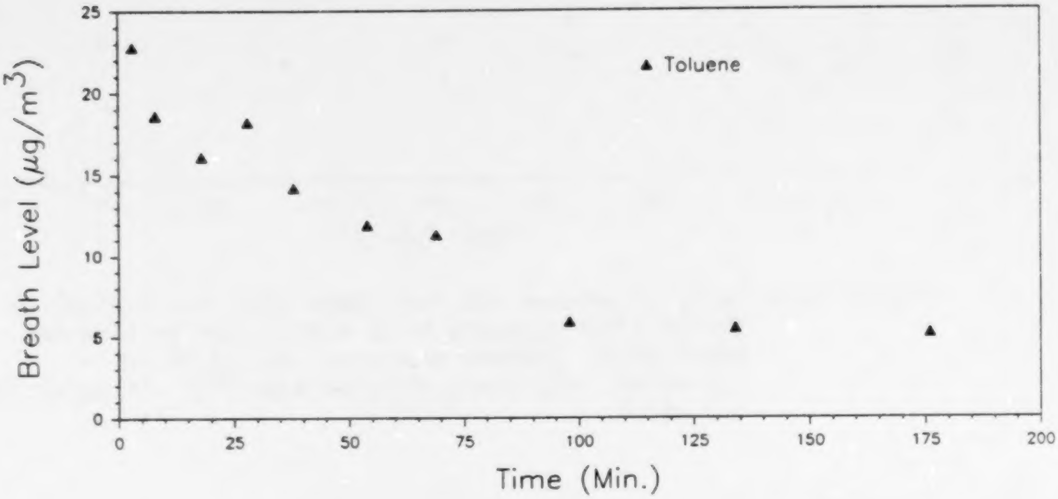

Figure E-16. Decay of toluene in alveolar breath after exposure to an active wood working and metal shop. Exposure: 510 $\mu g/m^3$; QL = 1.4 $\mu g/m^3$.

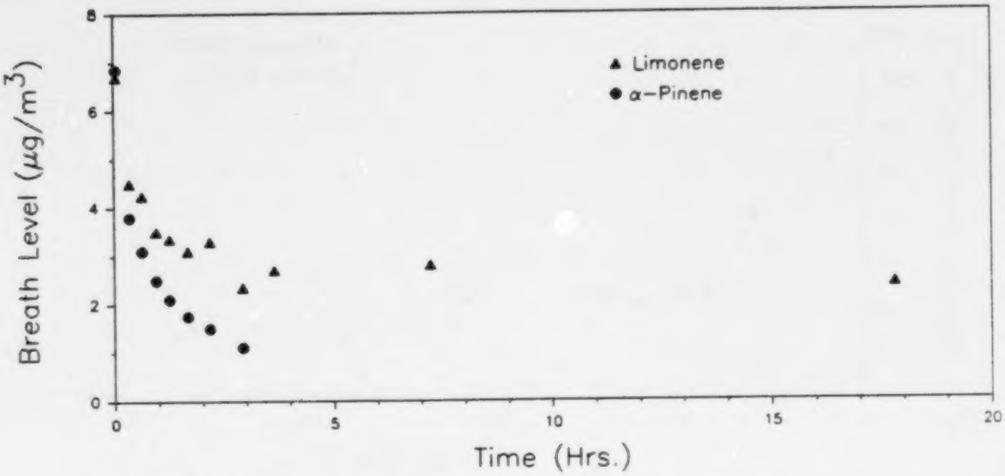

Figure E-17. Decay of limonene and α-pinene in whole breath after exposure to consumer products as determined by Tenax-based sampling and analysis. Limonene exposure: 160 $\mu g/m^3$, QL = 1.4 $\mu g/m^3$; α-pinene exposure: 95 $\mu g/m^3$; 1.1 $\mu g/m^3$.

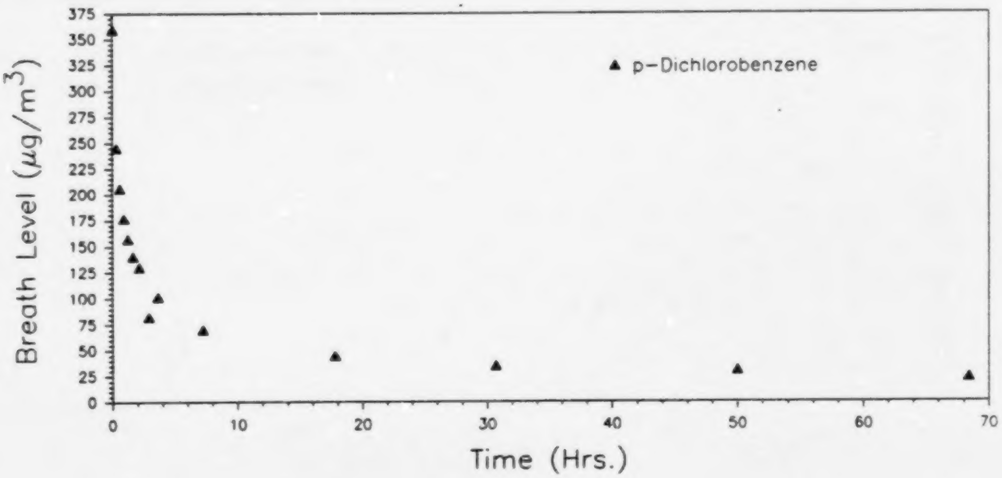

Figure E-18. Decay of p-dichlorobenzene in whole breath after exposure to consumer products as determined by Tenax-based sampling and analysis. Exposure: 10000 $\mu g/m^3$; QL = 4.6 $\mu g/m^3$.

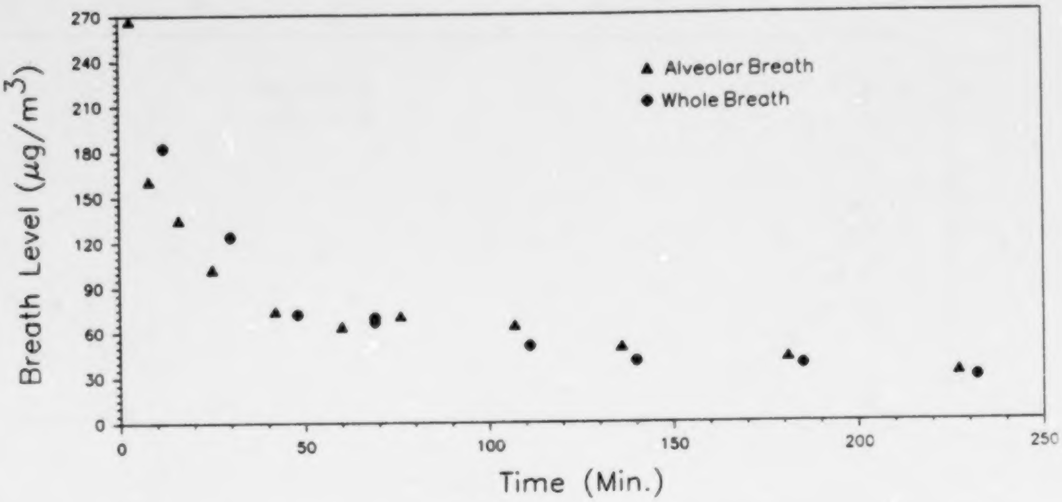

Figure E-19. Breath level of isopentane post exposure to staining in home garage. Exposure: 10,000 μg/m^3; QL = 3.3 μg/m^3.

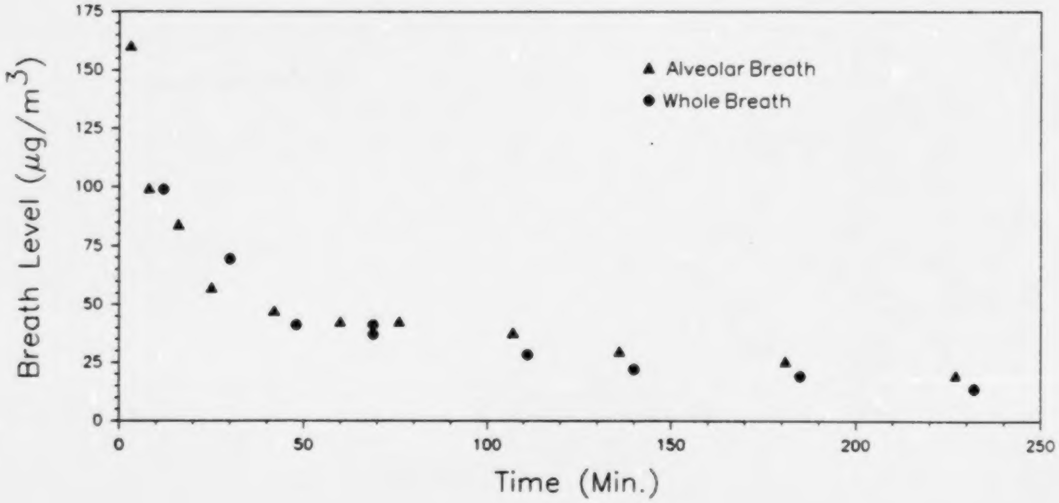

Figure E-20. Breath level of pentane post exposure to staining in home garage. Exposure: 3400 μg/m^3; QL = 0.4 μg/m^3.

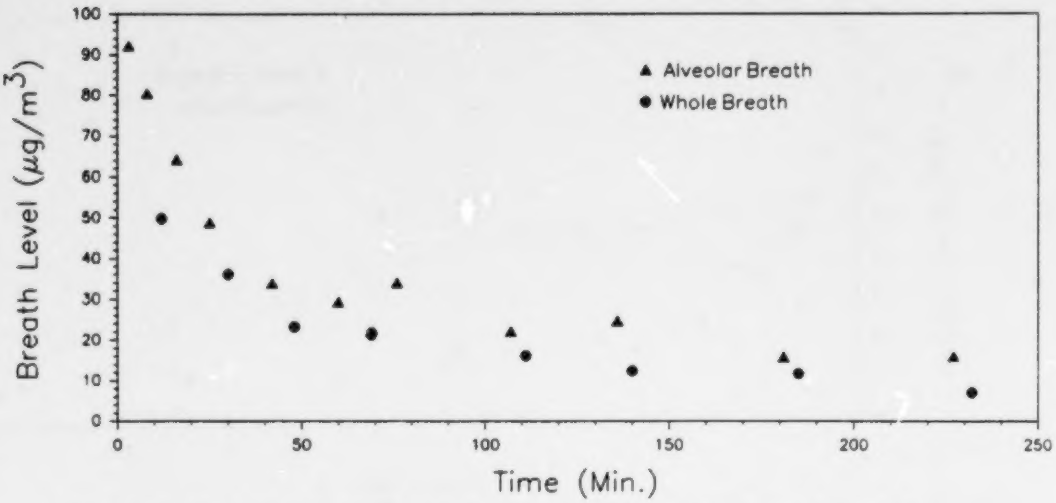

Figure E-21. Breath level of 2-methylpentane post exposure to staining in home garage. Exposure: 2000 µg/m^3; QL = 4.2 µg/m^3.

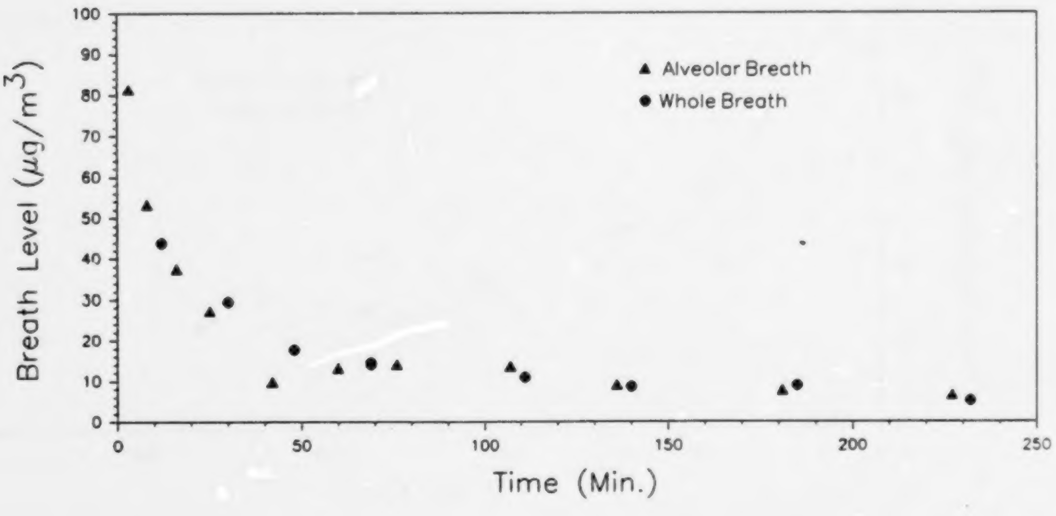

Figure E-22. Breath level of 2-methylhexane post exposure to staining in home garage. Exposure: 340 µg/m^3; QL = 0.9 µg/m^3.

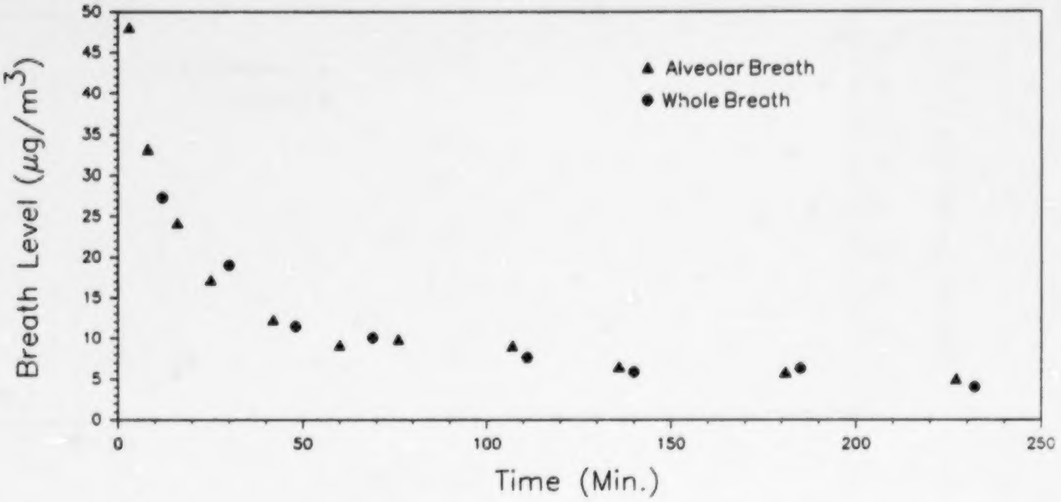

Figure E-23. Breath level of 3-methylhexane post exposure to staining in home garage. Exposure: 410 $\mu g/m^3$; QL = 0.9 $\mu g/m^3$.

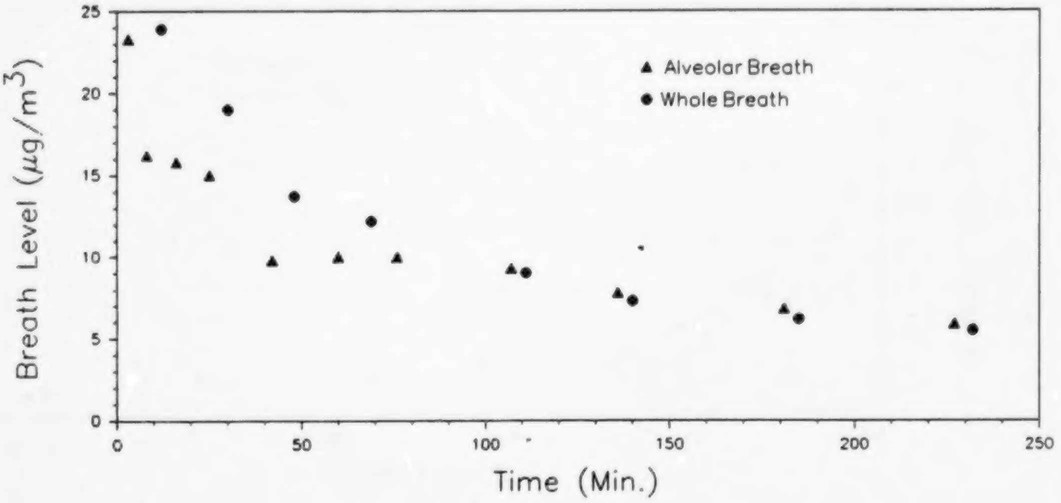

Figure E-24. Breath level of benzene post exposure to staining in home garage. Exposure: 430 $\mu g/m^3$; QL = 3.1 $\mu g/m^3$.

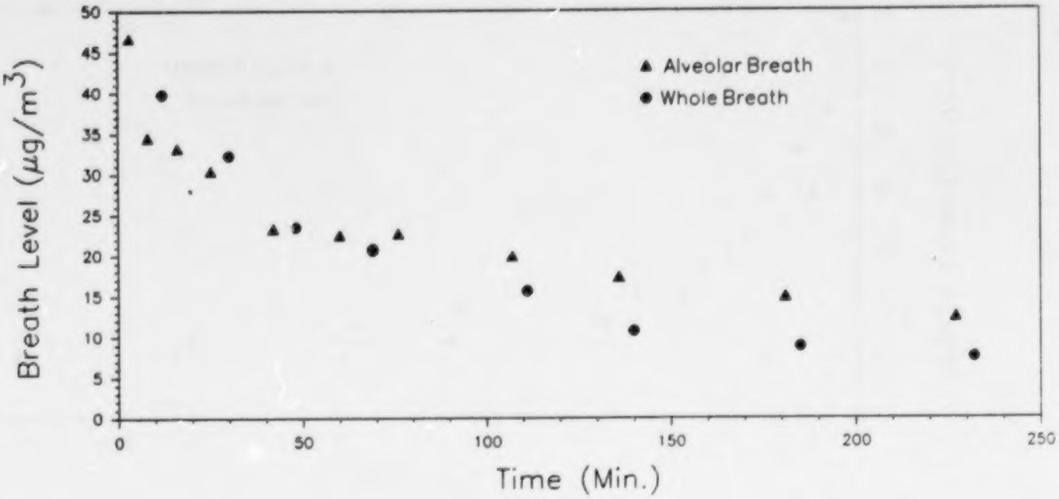

Figure E-25. Breath level of toluene post exposure to staining in home garage. Exposure: 1200 μg/m^3; QL = 1.1 μg/m^3.

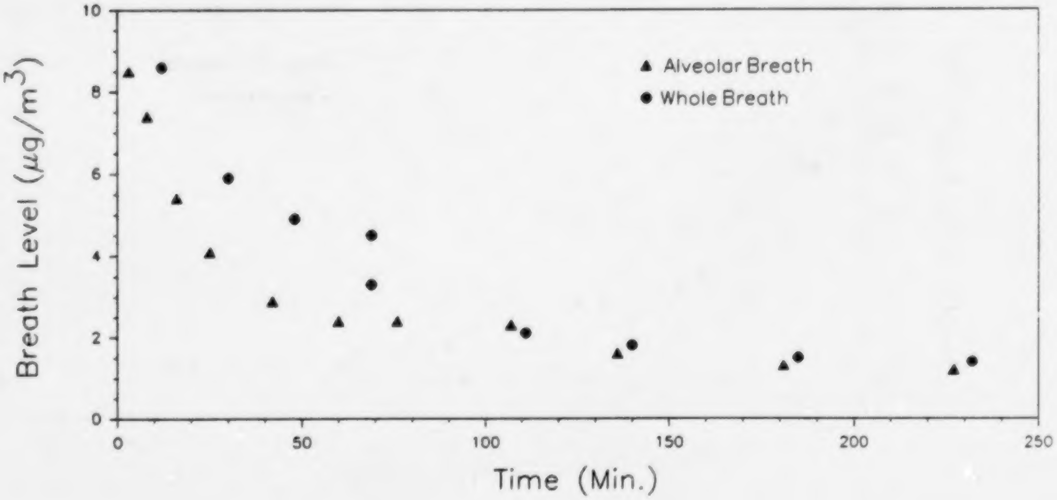

Figure E-26. Breath level of n-octane post exposure to staining in home garage. Exposure: 320 ng/L; QL = 0.9 μg/m^3.

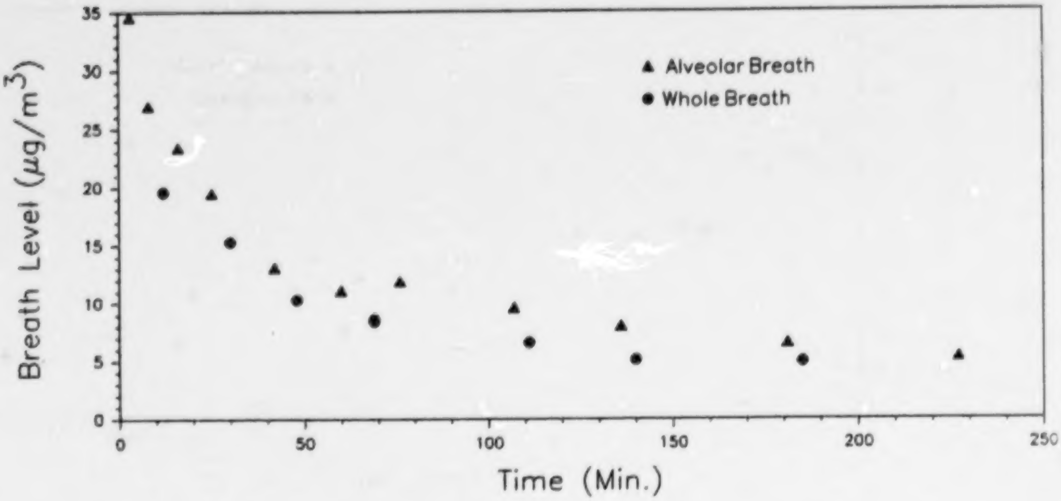

Figure E-27. Breath level of ethylcyclohexane post exposure to staining in home garage. Exposure: 900 μg/m³; QL = 4.2 μg/m³.

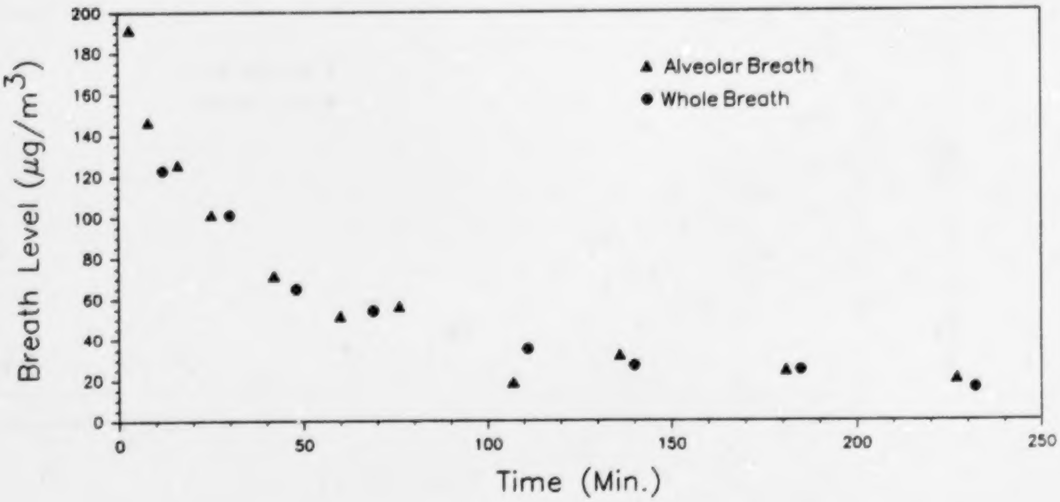

Figure E-28. Breath level of 3-methyloctane post exposure to staining in home garage. Exposure: 5400 μg/m³; QL = 0.9 μg/m³.

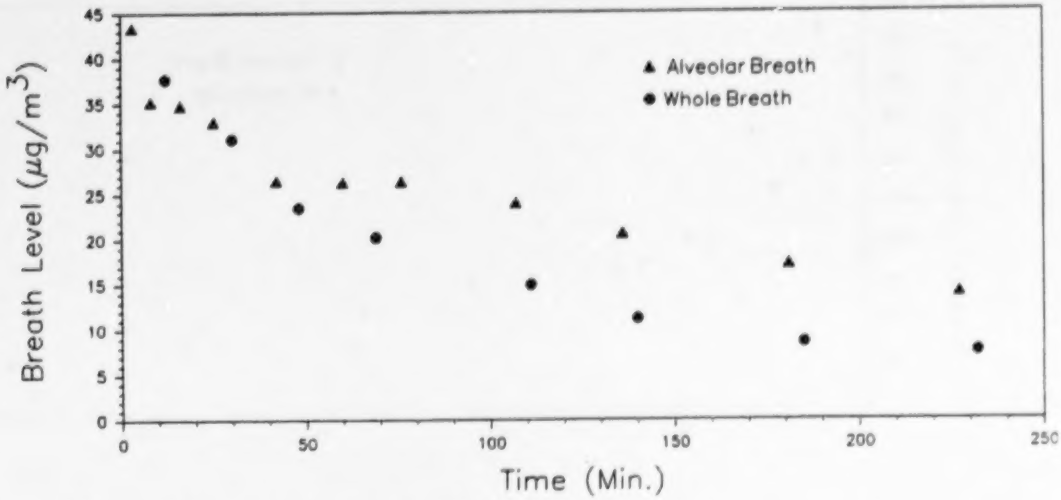

Figure E-29. Breath level of ethylbenzene post exposure to staining in home garage. Exposure: 2600 $\mu g/m^3$; QL = 0.7 $\mu g/m^3$.

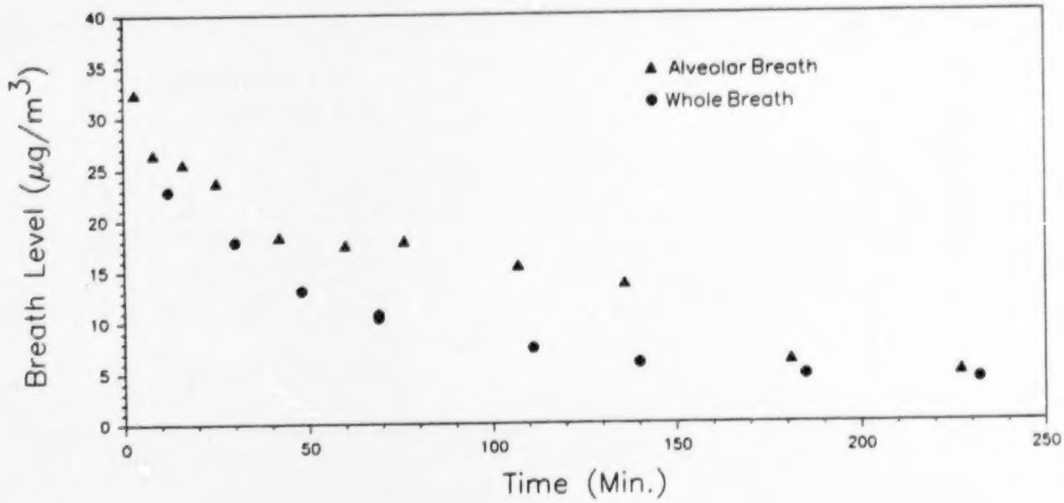

Figure E-30. Breath level of p-xylene post exposure to staining in home garage. Exposure: 1700 $\mu g/m^3$; QL = 0.5 $\mu g/m^3$.

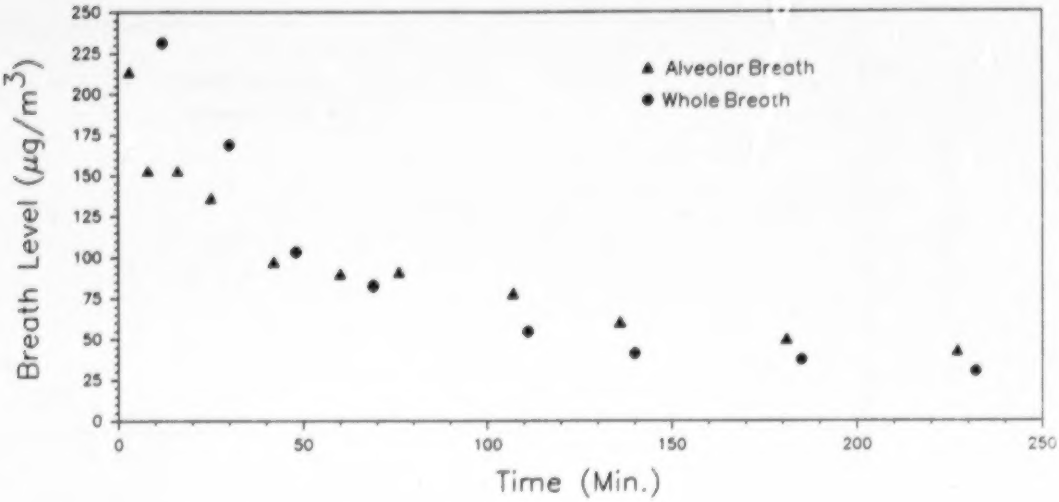

Figure E-31. Breath level of n-nonane post exposure to staining in home garage. Exposure: 12,000 $\mu g/m^3$; QL = 0.9 $\mu g/m^3$.

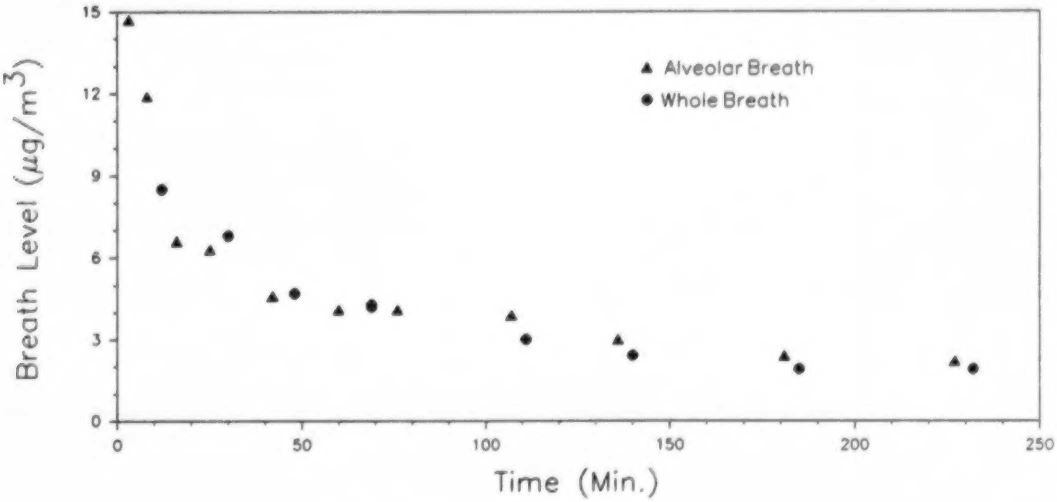

Figure E-32. Breath level of o-xylene post exposure to staining in home garage. Exposure: 700 $\mu g/m^3$; QL = 1.2 $\mu g/m^3$.

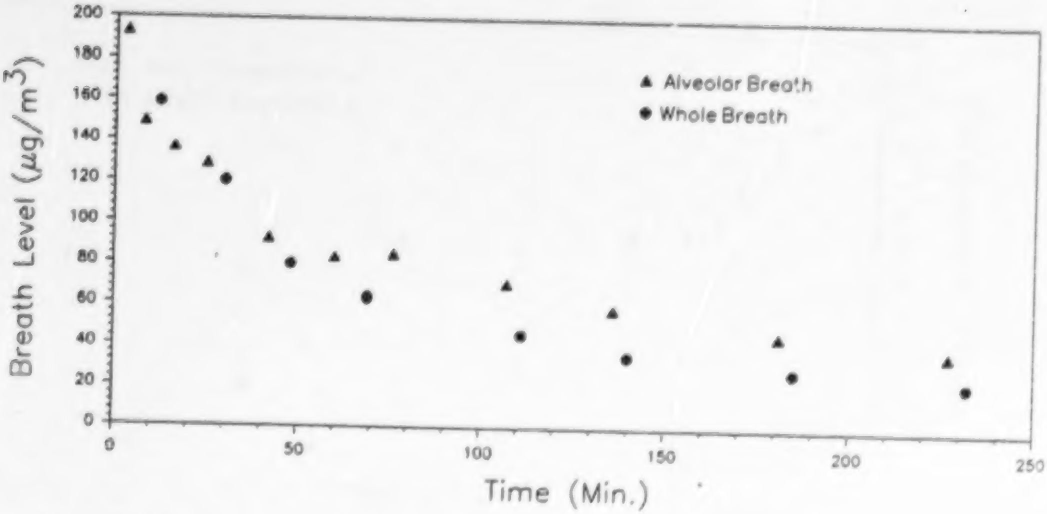

Figure E-33. Breath level of n-decane post exposure to staining in home garage. Exposure: 14,000 μg/m^3; QL = 1.3 μg/m^3.

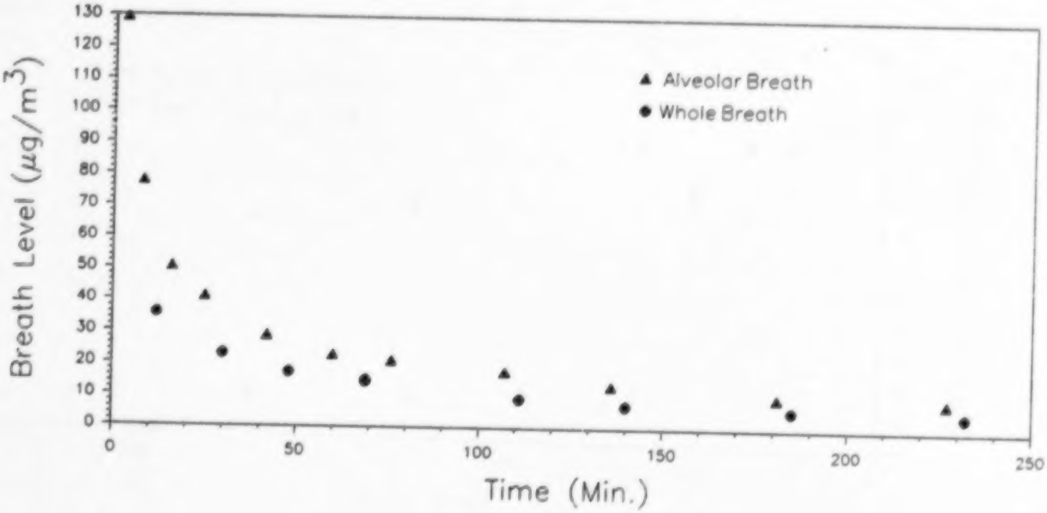

Figure E-34. Breath level of n-undecane post exposure to staining in home garage. Exposure: 5600 μg/m^3; QL = 1.3 μg/m^3.

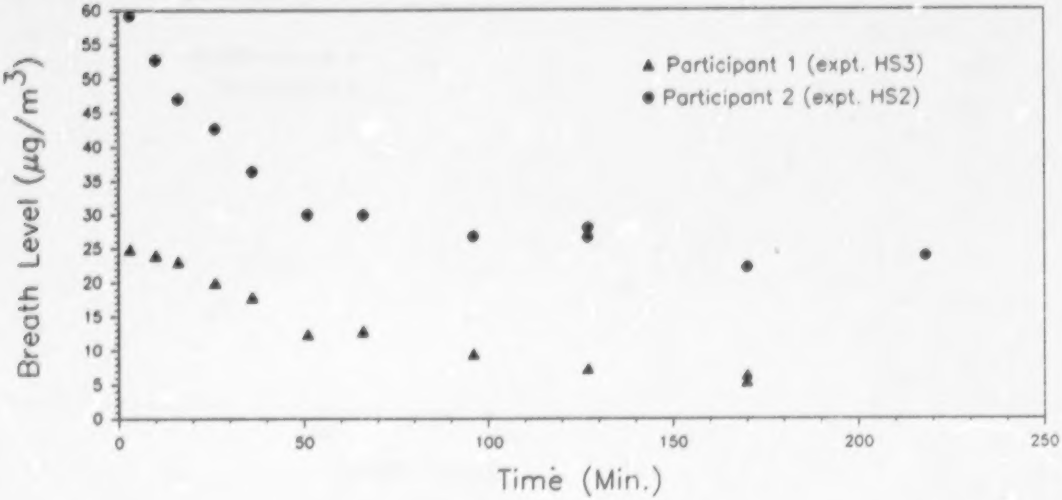

Figure E-35. Decay of dichloromethane in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 450 $\mu g/m^3$; QL = 6 $\mu g/m^3$.

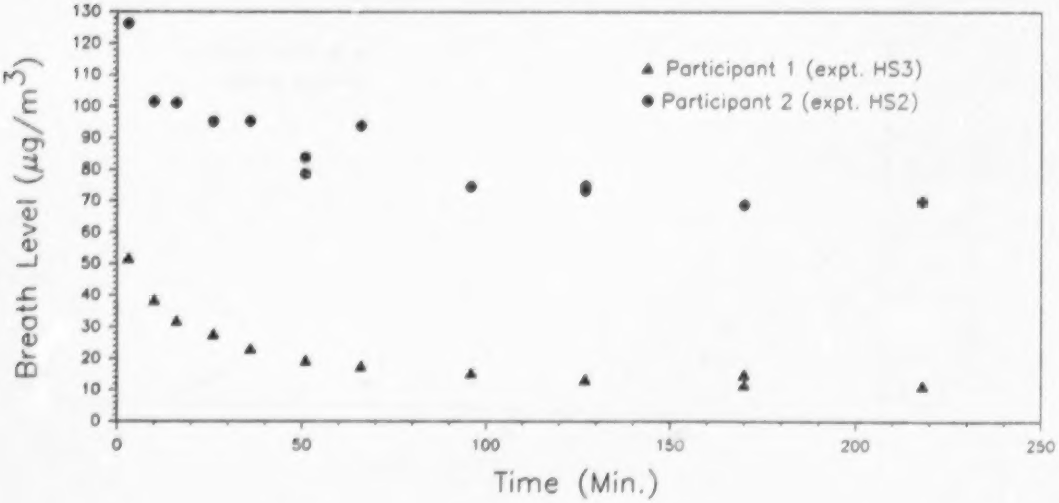

Figure E-36. Decay of 1,1,1-trichloroethane in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 200 $\mu g/m^3$; QL = 11 $\mu g/m^3$.

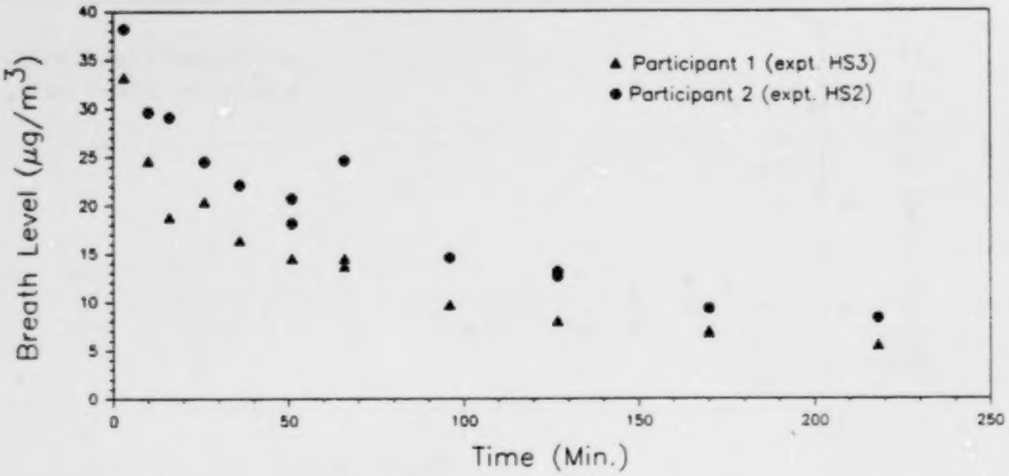

Figure E-37. Decay of toluene in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 640 µg/m³; QL = 1.4 µg/m³.

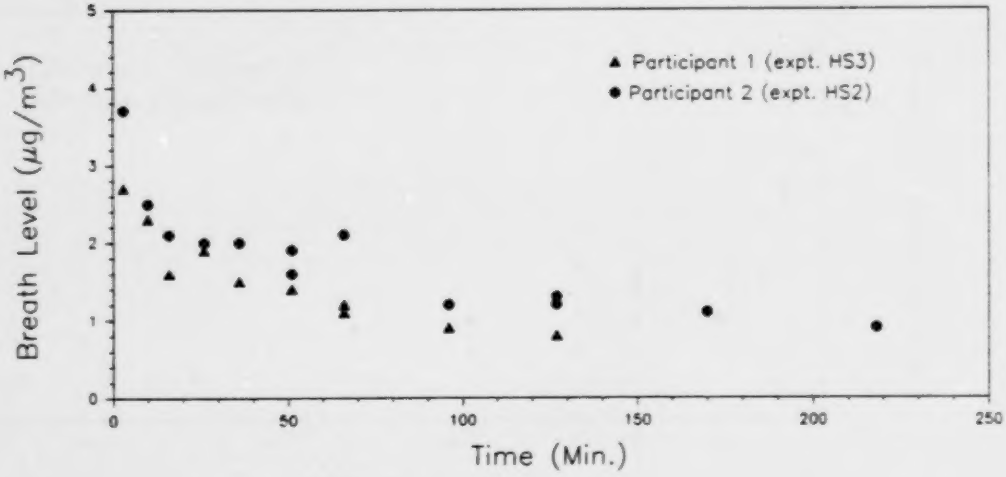

Figure E-38. Decay of ethylbenzene in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 150 µg/m³; QL = 0.9 µg/m³.

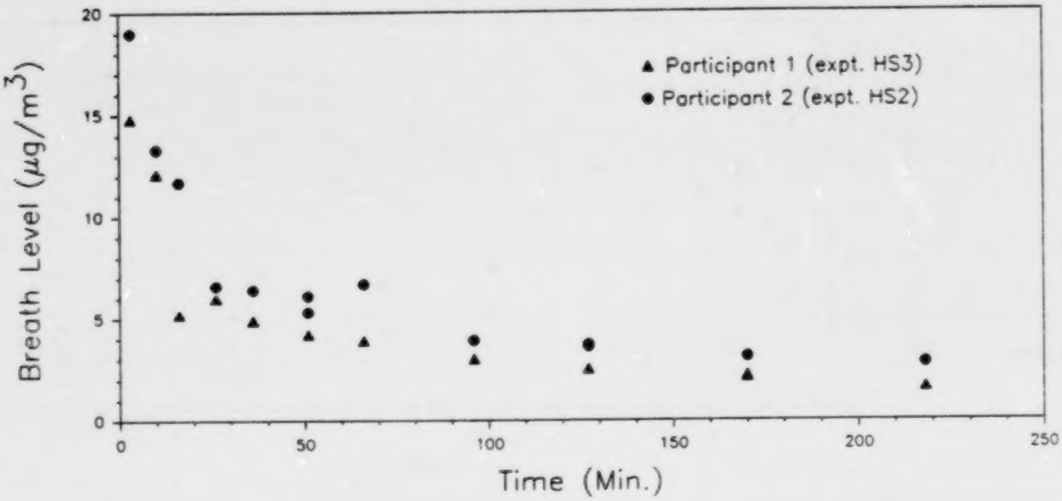

Figure E-39. Decay of p-xylene in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 570 µg/m³; QL = 0.7 µg/m³.

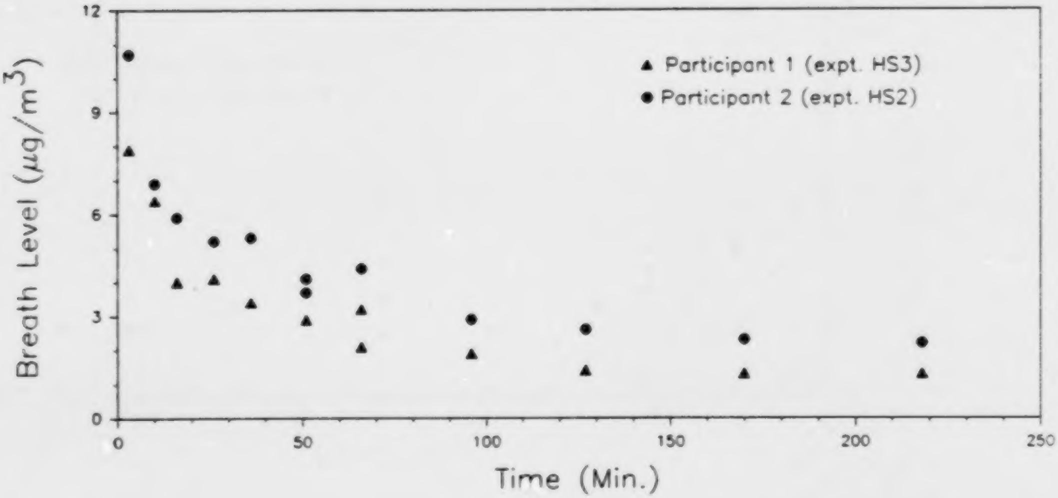

Figure E-40. Decay of n-nonane in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 200 µg/m³; QL = 1.2 µg/m³.

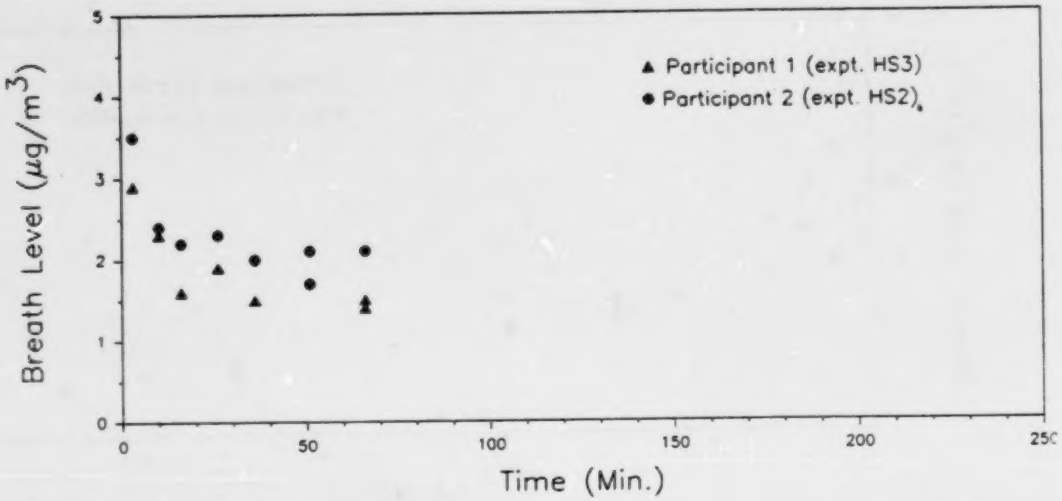

Figure E-41. Decay of o-xylene in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 200 µg/m^3; QL = 1.6 µg/m^3.

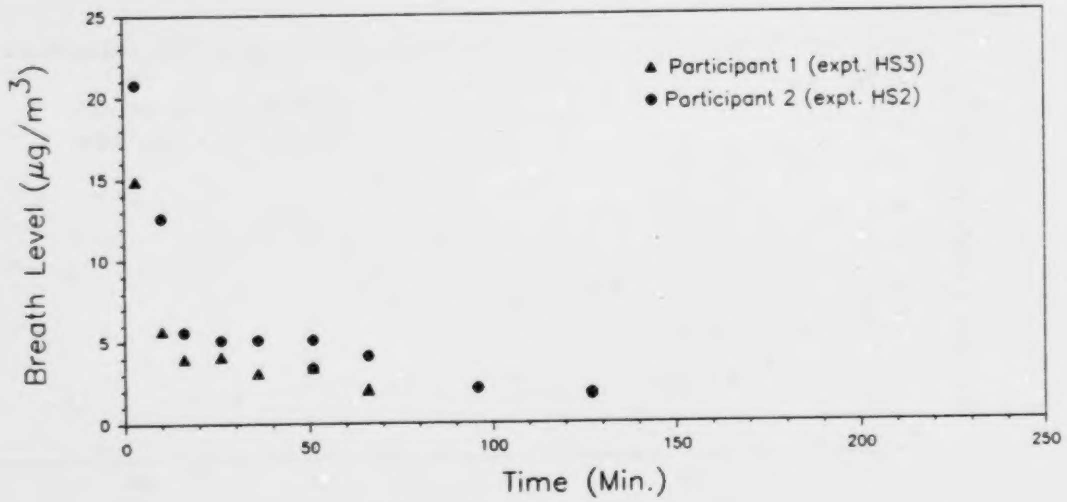

Figure E-42. Decay of n-decane in alveolar breath for two participants exposed at the same time in a hardware store environment. Exposure: 330 µg/m^3; QL = 1.7 µg/m^3.

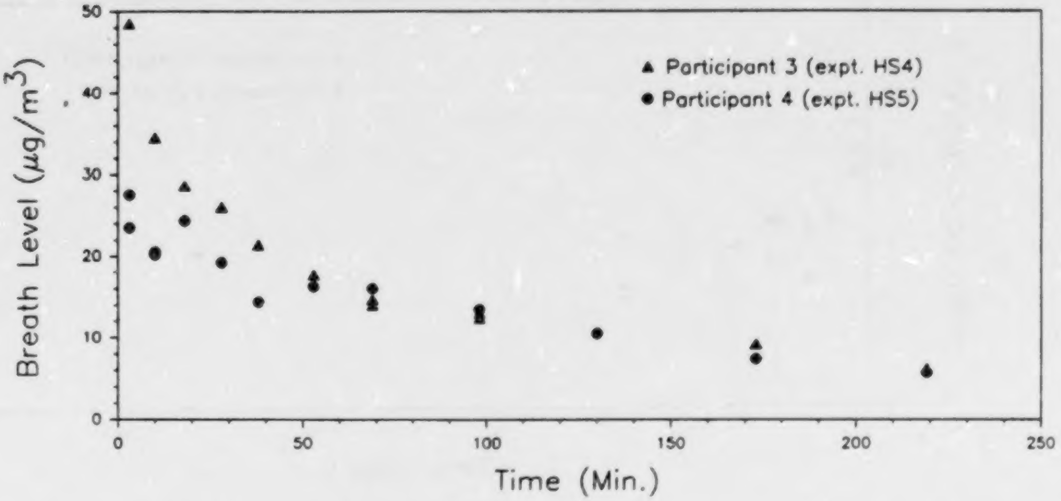

Figure E-43. Decay of dichloromethane in alveolar breath for two participants exposed at the same time in a hardware store environment. Mean exposure: 270 μg/m^3; QL = 6 μg/m^3.

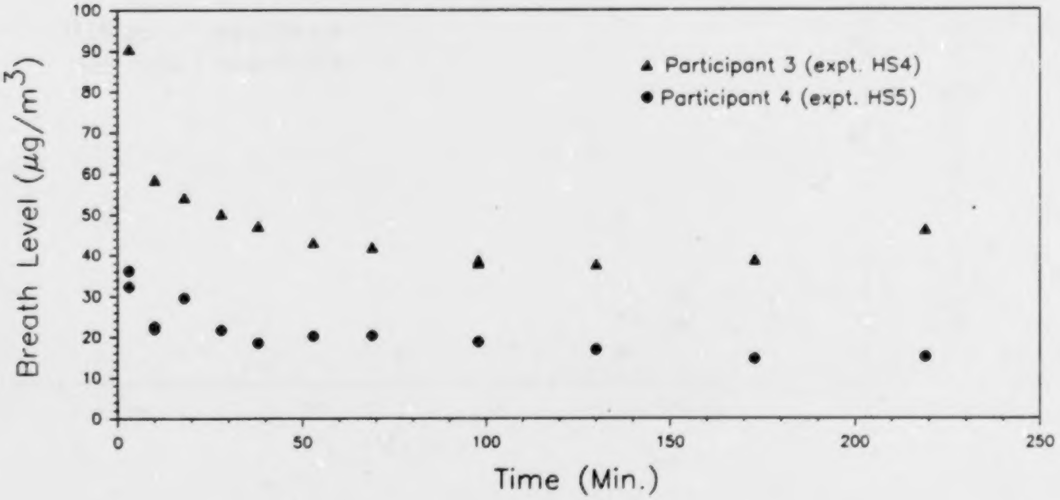

Figure E-44. Decay of 1,1,1-trichloroethane in alveolar breath for two participants exposed at the same time in a hardware store environment. Mean exposure: 210 μg/m^3; QL = 11 μg/m^3.

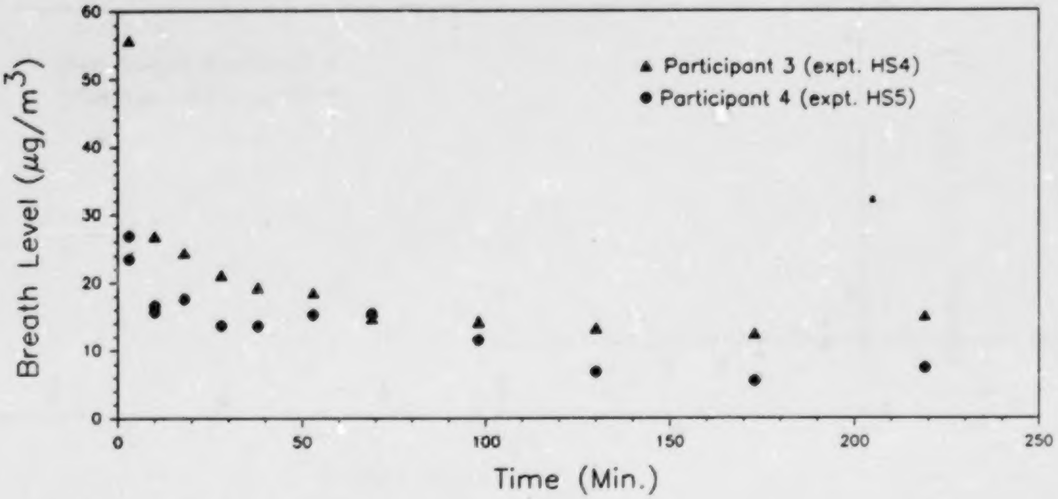

Figure E-45. Decay of toluene in alveolar breath for two participants exposed at the same time in a hardware store environment. Mean exposure: 370 $\mu g/m^3$; QL = 1.4 $\mu g/m^3$.

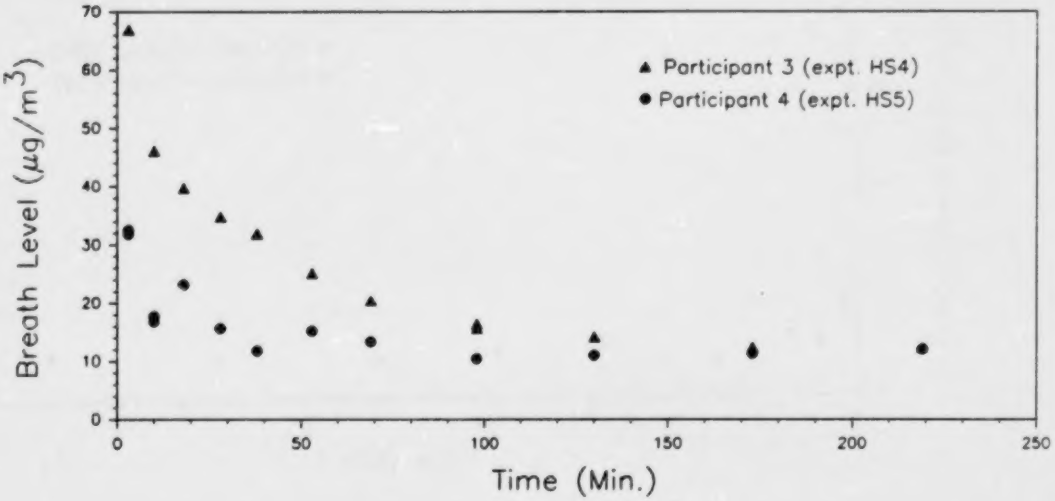

Figure E-46. Decay of tetrachloroethylene in alveolar breath for two participants exposed at the same time in a hardware store environment. Mean exposure: 170 $\mu g/m^3$; QL = 3.6 $\mu g/m^3$.

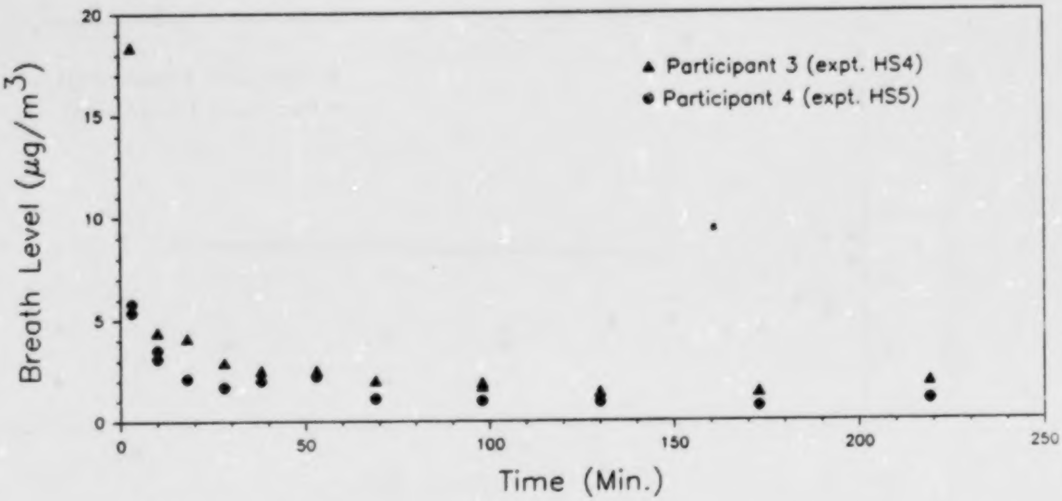

Figure E-47. Decay of p-xylene in alveolar breath for two participants exposed at the same time in a hardware store environment. Mean exposure: 190 $\mu g/m^3$; QL = 0.7 $\mu g/m^3$.

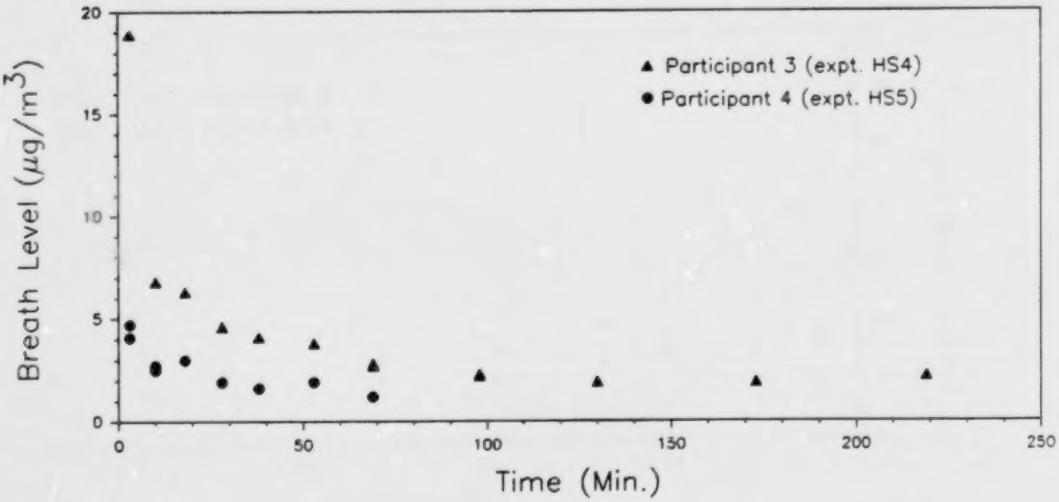

Figure E-48. Decay of n-nonane in alveolar breath for two participants exposed at the same time in a hardware store environment. Mean exposure: 120 $\mu g/m^3$; QL = 1.2 $\mu g/m^3$.

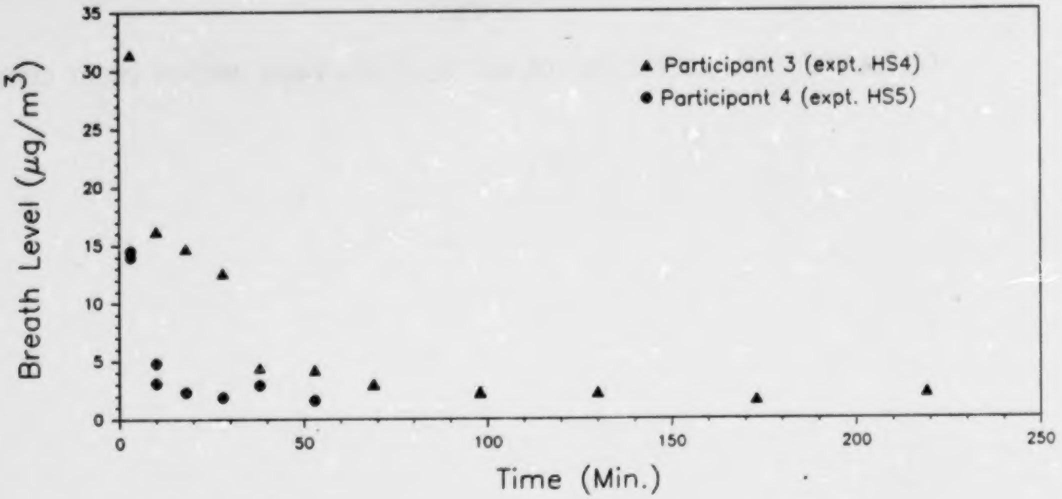

Figure E-49. Decay of n-decane in alveolar breath for two participants exposed at the same time in a hardware store environment. Mean exposure: 190 µg/m³; QL = 1.7 µg/m³.

APPENDIX F

CALCULATED HALF-LIFE DATA FOR ALVEOLAR AND WHOLE BREATH DECAY CURVES

TABLE F-1. CALCULATED HALF-LIVES FOR HALOGENATED HYDROCARBONS IN ALVEOLAR BREATH

Compound	Exposure[a] Conc. ug/m^3	Expt. Code	Partic-ipant	One Compartment Model: One Compart. t1/2 (h)	One Compartment Model: 95% Conf. Int. Range (h)	Two Compartment Model: First t1/2 (h)	Two Compartment Model: 95% Conf. Int. Range (h)	Two Compartment Model: Second t1/2 (h)	Two Compartment Model: 95% Conf. Int. Range (h)	r^2 One Compart	r^2 Two Compart.	Calculated $F_{2,d.f.}$	Best Compart. Fit (95% C.I.)
Halogenated Hydrocarbons													
Vinylidene chloride	56	WS1	1	2.97	1.70-11.6	0.12	0.07-3.25	11.60	3.85-NE[b]	0.962	0.994	18.2	2
Dichloromehtane	5000	FS1	1	0.60	0.43-1.02	0.13	0.10-0.25	1.80	1.25-3.22	0.964	0.998	50.8	2
Dichloromethane	470	HS1	2	0.40	0.30-0.62	0.10	0.07-0.15	1.07	0.82-1.53	0.971	0.998	61.9	2
Dichloromethane	460	HS3	1	1.07	0.91-1.31	0.78	0.23-NE	IC[c]	NC[d]	0.996	0.997	NC	NC
Dichloromethane	320	HS4	3	0.65	0.47-1.07	0.08	0.04-0.43	1.14	0.79-2.03	0.985	0.999	31.5	2
Dichloromethane	220	HS5	4	1.86	1.40-2.76	0.17	0.02-NE	2.07	1.15-10.0	0.987	0.988	0.3	1
Chloroform	600	SP1	2	0.72	0.52-1.17	0.08	0.05-0.22	1.58	1.10-2.63	0.968	0.997	36.4	2
1,1,1-Trichloroethane	16000	WS1	1	0.88	0.60-1.63	0.10	0.07-0.23	1.90	1.38-3.05	0.961	0.997	40.7	2
1,1,1-Trichloroethane	340	HS1	2	1.22	0.87-2.05	0.13	0.08-0.27	2.60	1.92-4.03	0.965	0.998	57.3	2
1,1,1-Trichloroethane	200	HS2	2	4.30	2.86-8.67	0.00	0.01-NE	3.81	0.03-NE	0.990	0.990	0.1	1
1,1,1-Trichloroethane	200	HS3	1	0.99	0.67-1.88	0.17	0.13-0.24	3.18	2.18-5.95	0.962	0.999	103.4	2
1,1,1-Trichloroethane	200	HS5	4	3.39	2.11-8.60	0.17	0.05-NE	6.08	2.20-NE	0.979	0.987	2.2	1
1,1,1-Trichloroethane	140	FS1	1	1.00	0.70-1.77	0.08	0.05-0.15	1.80	1.45-2.35	0.974	0.999	74.6	2
Trichloroethylene	77	FS1	1	0.65	0.45-1.19	0.20	0.06-0.20	IC	NC	0.987	0.998	NC	NC
Tetrachloroethylene	280	HS1	2	2.42	1.87-3.43	0.18	0.07-NE	3.70	2.23-10.8	0.989	0.996	6.5	2
Tetrachloroethylene	190	HS4	3	0.85	0.61-1.40	0.11	0.06-0.53	1.67	1.13-3.13	0.970	0.995	18.6	2
Tetrachloroethylene	150	HS5	4	2.06	1.11-15.6		Residual Convergance Failure			0.925	NC	NC	NC

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[a] Exposure concentrations for the garage experiment (GS1) are approximate.

[b] NE = Confidence interval included negative exponents which can't be transformed into half-life values using this method.

[c] IC = Model reflects insufficient change in concentration to calculate a second half-life over this time interval.

[d] NC = Not calculated.

TABLE F-2. CALCULATED HALF-LIVES FOR AROMATIC HYDROCARBONS IN ALVEOLAR BREATH

Compound	Exposure[a] Conc. ug/m3	Expt. Code	Participant	One Comparment Model		Two Compartment Model				r2 One Compart.	r^2 Two Compart.	Calculated $F_{2,d.f.}$	Best Compart. Fit (95% C.I.)
				One Compart. t1/2 (h)	95% Conf. Int. Range (h)	First t1/2 (h)	95% Conf. Int. Range (h)	Second t1/2 (h)	95% Conf. Int. Range (h)				
Aromatic Hydrocarbons													
Benzene	430	GS1	1	1.68	1.14-3.18	0.14	0.06-NE[b]	3.38	1.80-29.1	0.969	0.992	9.9	2
Toluene	5700	FS1	1	0.82	0.55-1.52	0.10	0.07-0.18	1.82	1.38-2.63	0.958	0.998	68.9	2
Toluene	1200	GS1	1	1.84	1.30-3.16	0.05	0.03-NE	2.64	1.96-4.04	0.977	0.996	18	2
Toluene	640	HS2	2	1.53	1.15-2.27	0.07	0.02-NE	1.88	1.33-3.26	0.986	0.993	4.1	1
Toluene	640	HS3	1	1.06	0.76-1.73	0.08	0.05-0.41	1.68	1.25-2.56	0.975	0.997	22	2
Toluene	510	WS1	1	1.15	0.92-1.55	Residual Convergence Failure				0.989	NC[c]	NC	NC
Toluene	460	HS4	3	1.13	0.60-8.83	0.05	0.03-0.11	4.05	2.41-12.8	0.995	0.995	4.7	2
Toluene	320	HS1	2	0.52	0.38-0.82	0.27	0.15-1.23	3.23	0.83-NE	0.967	0.989	8.4	2
Toluene	280	HS5	4	1.64	1.09-4.79	Residual Convergence Failure				0.967	NC	NC	NC
Ethylbenzene	2600	GS1	1	2.46	1.91-3.45	0.03	0.01-NE	2.90	2.28-4.00	0.992	0.997	7.1	2
Ethylbenzene	360	HS1	2	0.22	0.13-0.42	0.08	0.07-0.15	2.12	1.10-29.3	0.931	0.992	32.4	2
Ethylbenzene	150	HS2	2	1.70	1.11-3.61	0.04	0.02-NE	2.49	1.73-4.48	0.966	0.994	16.4	2
Ethylbenzene	150	HS3	1	1.02	0.72-1.72	0.08	0.02-NE	1.43	0.80-7.13	0.984	0.993	2.9	1
m,p-Xylene	1600	HS1	2	0.92	0.72-1.23	0.03	0.01-NE	1.10	0.88-1.45	0.983	0.995	9.4	2
m,p-Xylene	1700	GS1	1	1.60	1.27-2.17	Residual Convergence Failure				0.990	NC	NC	NC
m,p-Xylene	560	HS2	2	0.64	0.41-1.38	0.13	0.08-0.37	2.42	1.23-60.5	0.943	0.992	22.2	2
m,p-Xylene	560	HS3	1	0.45	0.28-1.13	0.11	0.06-1.05	2.15	0.88-NE	0.922	0.980	10.3	2
m,p-Xylene	230	HS4	3	0.08	0.05-0.23	0.03	0.02-0.06	2.16	1.24-8.75	0.895	0.995	68.9	2
m,p-Xylene	160	HS5	4	0.58	0.35-1.62	0.08	0.05-0.56	2.12	1.07-86.2	0.915	0.985	16.3	2
o-Xylene	440	HS1	2	0.25	0.15-0.58	0.08	0.04-NE	1.17	0.35-NE	0.941	0.983	6	1
o-Xylene	700	GS1	1	0.67	0.42-1.69	0.11	0.08-0.20	2.94	1.69-11.2	0.927	0.996	56.1	2
o-Xylene	190	HS2	2	1.61	0.73-7.86	0.04	0.02-NE	9.95	1.83-NE	0.979	0.999	30.8	2

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[a] Exposure concentrations for the garage experiment (GS1) are approximate.

[b] NE = Confidence interval included negative exponents which can't be transformed into half-life values using this method.

[c] NC = Not calculated.

TABLE F-3. CALCULATED HALF-LIVES FOR ALIPHATIC HYDROCARBONS IN ALVEOLAR BREATH

				One Compartment Model		Two Compartment Model							
Compound	Exposure[a] Conc. ug/m^3	Expt. Code	Partic-ipant	One Compart. t1/2 (h)	95% Conf. Int. Range (h)	First t1/2 (h)	95% Conf. Int. Range (h)	Second t1/2 (h)	95% Conf. Int. Range (h)	r2 One Compart.	r2 Two Compart.	Calculated $F_{2,d.f.}$	Best Compart. Fit (95% C.I.)
Aliphatic Hydrocarbons, Straight-Chain													
n-Pentane	3400	GS1	1	0.70	0.43-1.81	0.08	0.06-0.16	2.34	1.51-5.13	0.925	0.966	58.5	2
n-Pentane	340	WS1	1	1.15	0.60-17.2	0.07	0.01-NE[b]	2.07	0.48-0.90	0.954	0.967	0.8	1
n-Octane	320	GS1	1	0.67	0.47-1.16	0.19	0.14-0.28	2.84	1.74-7.70	0.962	0.999	75.3	2
n-Octane	39	HS2	2	0.87	0.54-2.30	0.17	0.04-NE	IC[c]	NC[d]	0.985	0.995	NC	NC
n-Nonane	12000	GS1	1	1.37	1.01-2.15	0.02	0.01-NE	1.73	1.31-2.55	0.978	0.994	8.9	2
n-Nonane	210	HS2	2	1.13	0.74-2.36	0.06	0.04-0.18	2.01	1.50-3.02	0.958	0.997	42.4	2
n-Nonane	210	HS3	1	0.68	0.47-1.23	0.15	0.08-0.82	2.06	1.05-6.12	0.961	0.992	13.1	2
n-Nonane	180	HS1	2	0.08	0.05-6.33	0.02	0.01-0.17	0.48	0.30-1.17	0.918	0.999	109.0	2
n-Nonane	130	HS4	3	0.21	0.13-0.58	0.04	0.02-0.10	1.53	0.97-3.53	0.886	0.993	56.5	2
n-Nonane	110	HS5	4	0.61	0.39-1.46	Residual Conv^rgence Failure				0.978	NC	NC	NC
n-Decane	14000	GS1	1	1.35	1.03-1.96	0.18	0.092-3.89	2.33	1.55-4.95	0.984	0.997	13.8	2
n-Decane	360	HS2	2	0.22	0.14-0.57	0.08	0.04-0.81	1.39	0.47-NE	0.927	0.987	11.1	2
n-Decane	360	HS3	1	0.17	0.09-1.10	0.04	0.02-NE	1.06	0.43-NE	0.911	0.997	51.0	2
n-Decane	260	HS1	2	0.08	0.07-0.17	0.07	0.02-NE	IC	NC	0.990	0.999	NC	NC
n-Decane	210	HS4	3	0.27	0.20-0.44	0.19	0.10-1.24	2.82	0.41-0.58	0.962	0.974	1.6	1
n-Decane	170	HS5	4	0.11	0.06-0.74	0.05	0.03-NE	IC	NC	0.938	0.997	NC	NC
n-Undecane	5600	GS1	1	0.28	0.18-0.58	0.07	0.06-0.10	1.36	1.04-1.95	0.941	0.999	142.0	2
Aliphatic Hydrocarbons, Branched-Chain													
Isopentane	10000	GS1	1	0.65	0.40-1.77	0.08	0.05-0.19	2.33	1.38-7.45	0.920	0.993	37.5	2
2-Methylpentane	2000	GS1	1	0.86	0.60-1.48	0.21	0.14-0.42	3.18	1.67-35.2	0.965	0.997	35.9	2
2-Methylhexane	340	GS1	1	0.26	0.17-0.49	0.13	0.09-0.21	3.16	1.25-NE	0.948	0.994	26.2	2
3-Methylhexane	410	GS1	1	0.39	0.26-0.77	0.13	0.10-0.17	2.54	1.62-5.88	0.946	0.998	101.0	2
3-Methylhexane	39	FS1	1	0.42	0.30-0.65	Residual Convergence Failure				0.993	NC	NC	NC
2-Methyloctane	5400	GS1	1	0.60	0.46-0.85	0.28	0.16-1.07	2.48	0.85-NE	0.981	0.995	8.7	2
Ethylcyclohexane	900	GS1	1	0.89	0.64-1.48	0.19	0.12-0.40	2.53	1.53-7.36	0.969	0.997	34.3	2

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[a] Exposure concentrations for the garage experiment (GS1) are approximate.

[b] NE = Confidence interval included negative exponents which can't be transformed into half-life values using this method.

[c] IC = Model reflects insufficient change in concentration to calculate a second half-life over this time interval.

[d] NC = Not calculated.

TABLE F-4. CALCULATED HALF-LIVES FOR AROMATIC AND HALOGENATED HYDROCARBONS IN WHOLE BREATH

Compound	Exposure[a] Conc. ug/m^3	Expt. Code	Partic-ipant	One Compartment Model		Two Compartment Model							
				One Compart. t1/2 (h)	95% Conf. Int. Range (h)	First t1/2 (h)	95% Conf. Int. Range (h)	Second t1/2 (h)	95% Conf. Int. Range (h)	r^2 One Compart.	r^2 Two Compart.	Calculated $F_{2,d.f.}$	Best Compart. Fit (95% C.I.)
Aromatic Hydrocarbons													
Benzene	430	GS1	1	1.30	1.01-1.82	0.46	0.29-1.08	4.12	1.75-NE[b]	0.988	0.999	44.9	2
Toluene	5700	FS1	1	1.03	0.82-1.38	0.32	0.23-0.45	2.28	1.60-3.48	0.987	0.999	123	2
Toluene	1200	GS1	1	1.24	1.01-1.58	0.31	0.12-NE	1.86	1.06-7.75	0.977	0.998	6.5	2
Toluene	320	HS1	2	1.03	0.75-1.57	Residual Convergence Failure				0.976	NC[d]	NC	NC
Ethylbenzene	2600	GS1	1	1.25	1.05-1.56	0.48	0.22-NE	2.45	1.02-NE	0.994	0.999	10.9	2
Ethylbenzene	360	HS1	2	0.95	0.13-0.72	0.25	0.15-0.73	2.17	1.32-6.20	0.979	0.998	28.7	2
m,p-Xylene	1600	HS1	2	1.05	0.83-1.42	0.18	0.07-NE	1.60	1.05-3.32	0.986	0.997	10	2
m,p-Xylene	1700	GS1	1	1.06	0.85-1.42	0.52	0.33-1.28	4.98	1.28-2.62	0.989	0.999	27.9	2
m,p-Xylene	240	FS1	1	0.55	0.42-0.82	0.25	0.20-0.37	2.52	1.33-20.9	0.973	0.999	70.8	2
o-Xylene	440	HS1	2	0.93	0.68-1.47	0.08	0.03-NE	1.48	1.18-1.97	0.985	0.999	112	2
o-Xylene	700	GS1	1	1.21	0.94-1.68	0.53	0.28-NE	6.02	0.28-9.47	0.987	0.998	13.1	2
Halogenated Hydrocarbons													
Dichloromethane	5000	FS1	1	0.95	0.72-1.45	0.40	0.25-1.25	7.98	1.28-NE	0.975	0.997	17.1	2
Dichloromethane	470	HS1	2	0.55	0.45-0.75	0.33	0.28-0.45	5.40	1.67-4.35	0.982	0.999	58.4	2
1,1,1-Trichloroethane	340	HS1	2	1.33	1.00-2.07	1.38	0.30-2.67	IC[c]	NC	0.981	0.998	NC	NC
1,1,1-Trichloroethane	140	FS1	1	1.10	0.87-1.52	0.52	0.30-1.85	IC	NC	0.989	0.999	NC	NC
Tetrachloroethylene	280	HS1	2	2.13	1.45-4.02	1.68	0.07-0.07	IC	NC	0.980	0.982	NC	NC
p-Dichlorobenzene	9400	CP1	2	1.57	1.11-2.62	0.53	0.40-0.81	21.00	13.0-58.2	0.957	0.994	29.6	2

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[a] Exposure concentrations for the garage experiment (GS1) are approximate.

[b] NE = Confidence interval included negative exponents which can't be transformed into half-life values using this method.

[c] IC = Model reflects insufficient change in concentration to calculate a second half-life over this time interval.

[d] NC = Not calculated.

TABLE F-5. CALCULATED HALF-LIVES FOR ALIPHATIC AND CYCLIC HYDROCARBONS IN WHOLE BREATH

Compound	Exposure[a] Conc. ug/m^3	Expt. Code	Partic-ipant	One Compartment Model: One Compart. t1/2 (h)	One Compartment Model: 95% Conf. Int. Range (h)	Two Compartment Model: First t1/2 (h)	Two Compartment Model: 95% Conf. Int. Range (h)	Two Compartment Model: Second t1/2 (h)	Two Compartment Model: 95% Conf. Int. Range (h)	r^2 One Compart.	r^2 Two Compart.	Calculated $F_{2,d.f.}$	Best Compart. Fit (95% C.I.)
Aliphatic Hydrocarbons, Straight-Chain													
n-Pentane	3400	GS1	1	0.88	0.64-1.41	0.26	0.13-4.13	2.32	1.10-NE	0.973	0.996	15.3	2
n-Octane	320	GS1	1	0.95	0.74-1.32	0.00	0.42-NE[b]	0.61	0.27-NE	0.985	0.994	3.2	1
n-Nonane	12000	GS1	1	0.74	0.57-1.05	0.42	0.25-1.23	5.55	0.92-NE	0.982	0.997	13.6	2
n-Decane	14000	GS1	1	0.88	0.69-1.22	0.00	0.00-0.00	0.88	0.68-1.22	0.986	0.986	0	1
n-Undecane	5600	GS1	1	0.86	0.65-1.24	0.19	0.12-0.60	1.61	1.17-2.60	0.982	0.999	34.1	2
Aliphatic Hydrocarbons, Branched-Chain													
Isopentane	10000	GS1	1	0.89	0.62-1.50	0.24	0.14-0.81	2.05	1.40-NE	0.965	0.997	28.2	2
2-Methylpentane	2000	GS1	1	1.02	0.75-1.60	0.26	0.13-NE	2.25	1.17-NE	0.978	0.997	16.6	2
2-Methylhexane	340	GS1	1	0.87	0.60-1.52	0.29	0.16-1.64	3.47	1.22-NE	0.966	0.996	17.9	2
3-Methylhexane	400	GS1	1	0.88	0.63-1.46	0.31	0.19-0.87	3.57	1.39-NE	0.971	0.998	28.4	2
2-Methyloctane	5400	GS1	1	0.96	0.77-1.26	0.57	0.27-NE	5.20	0.57-NE	0.990	0.997	5.5	1
Cyclic Hydrocarbons													
Ethylcyclohexane	900	GS1	1	0.99	0.73-1.56	0.40	0.21-3.96	6.64	1.00-NE	0.983	0.998	19.8	2
α-Pinene	97	CP1	2	0.79	0.56-1.35	0.13	0.04-0.22	1.60	1.29-6.90	0.972	0.999	163.8	2
Limonene	160	CP1	2	2.43	1.56-5.49	0.24	0.11-NE	6.88	2.54-NE	0.976	0.996	2.01	1

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[a] Exposure concentrations for the garage experiment (GS1) are approximate.

[b] NE = Confidence interval included negative exponents which can't be transformed into half-life values using this method.